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by Kazem Omidvar

Goddard Space Flight Center
Greenbelt, Maryland

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SUMMARY

A numerical calculation has been carried out to evaluate the 3x3 cross-section matrix involved in the electron impact excitation of the ground state of H atom to the 2s and 2p levels. The method of solution is that of atomic eigenstates expansion. In this paper, instead of the iterative technique used by other authors, the definite integral terms in the coupled radial differential equations are eliminated through some linear transformation of the radial functions, thus avoiding iteration of these equations. The accuracy of the numerical integration is tested by satisfying the equation of reciprocity and the equation of continuity of currents with an error-to-value ratio less than 1 per 1000 on the average; and the maximum of this ratio, except for a few cases, has been kept below 5 percent. The results are in agreement with the results of an iterative technique.

To evaluate the effect of the long-range and the centrifugal potential, a simple perturbation theory is developed. The six cross sections $1s \rightarrow 2s$, $1s \rightarrow 2p$, $1s \rightarrow 1s$, $2s \rightarrow 2s$, $2s \rightarrow 2p$, and $2p \rightarrow 2p$ are tabulated. The $2p \rightarrow 2p$ cross section requires the solution of the sets of differential equations with different parities. With the validity of the eigenstates expansion assumed, it is found by comparison with the eigenstates expansion calculation that the Born approximation, despite its simplicity, gives meaningful results for low and close-to-the-threshold energies of the bombarding electrons. The effect of the exchange potentials on the cross sections is also investigated. Finally, an interesting structure of the $1s \rightarrow 2s$ excitation cross section above threshold is found.

CONTENTS

THEORY OF THE 2s AND 2p EXCITATION OF THE HYDROGEN ATOM INDUCED BY ELECTRON IMPACT*

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INTRODUCTION

Calculation of the excitation cross sections in atomic hydrogen by electron impact corresponds to the solution of the problem of three interacting bodies: one proton, and two electrons. By taking the position of the proton as the center of mass, the problem will reduce to the task of finding the nonseparable wave function of the system of the two electrons with an attractive center of force. Such a solution has not been found. However, if this wave function is expanded in terms of the eigenstates of the hydrogen atom, the coefficients of the expansion, which are functions of the position vector of the free electron, can be found through numerical integration. When an infinite number of terms is included in the expansion, the solution to the problem is exact. Furthermore, the expansion has the advantage that the asymptotic form of its coefficients is automatically the asymptotic form of the free electron wave function scattered from different atomic states, which are simply related to the excitation cross sections.

In this paper, atomic states 1s, 2s, 2p are included in the expansion and, by antisymmetrizing the two electron wave functions according to the exclusion principle, some contribution from the continuum in the expansion is also taken into account. The first calculation of this type was performed by Marriot (Reference 1), whose expansion consisted of the 1s and the 2s states in order to calculate the 1s → 2s transition cross section. This calculation was extended by Smith (Reference 2) to higher total orbital angular momenta of the system. Percival and Seaton (Reference 3) have formulated the eigenstate expansion technique in general and have tabulated the coefficients of the integro-differential equations for s, p, and d atomic electrons. Burke, Smith, and Schey (References 4 and 5†), using the equations of Percival and Seaton for the three states 1s, 2s, 2p, have integrated the resulting integro-differential equations. In this paper we solve the same differential equations by a linear transformation of the differential equations in order to avoid the need for iteration of these equations (Reference 6).‡

*Also has appeared in a condensed form in the *Physical Review*, Vol. 133, Feb. 17, 1964.

†A similar calculation has been performed by R. Damburg and R. Peterkop; this will appear in the *USSR Journal of Experimental and Theoretical Physics*. A different method to calculate the 1s-2s electron impact transition cross section in hydrogen is being considered by L. Kyle and A. Temkin, adopting the nonadiabatic theory of electron scattering developed by A. Temkin (see References 21, 22); the calculation is in progress.

‡A similar calculation has been carried out in Reference 6. Here the L = 0,1 cases have been solved by noniterative, and all other cases by iterative, methods.

The numerical integrations were carried out for all partial waves, while in higher partial waves the Born approximation was used. The transition between the eigenstates expansion calculation and the Born approximation takes place when the results of the two calculations agree closely.

FORMULATION

Derivation of the Differential Equations

Since spin orbit interaction of the electrons is neglected, the total orbital angular momentum L and the total spin angular momentum S are separately conserved. We can then divide the interactions into antiparallel spin states, where $S = 0$, and parallel spin states, where $S = 1$. We deal with spatial wave functions of the electrons only, and for brevity we call the orbital angular momentum the *angular momentum.*

Neglecting the motion of the proton of the hydrogen atom and taking its position as the origin of the coordinate system, the Schroedinger equation for the system can be written

$$[H - E]\,\psi(\mathbf{r}_1, \mathbf{r}_2) = 0 \,, \tag{1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the bound and free electrons; and in atomic units

$$H - E = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E \,, \tag{2}$$

where E is the total energy of the system and r_{12} is the distance between the two electrons. We expand the total wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ in terms of the eigenfunctions of the total angular momentum L,

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L=0}^{\infty} \psi_L(\mathbf{r}_1, \mathbf{r}_2) \,. \tag{3}$$

Since these eigenfunctions are orthogonal and distinct, substitution of Equation 3 in Equation 1 gives

$$[H - E]\,\psi_L(\mathbf{r}_1, \mathbf{r}_2) = 0 \,. \tag{4}$$

The explicit form of $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ is given by

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = (1+\beta P_{12}) \sum_{n_1 \ell_1 \ell_2} \sum_{m_1 m_2} C^{\ell_1 \ell_2 L}_{m_1 m_2 M} \phi(n_1 \ell_1 m_1, \mathbf{r}_1)$$

$$\times\ r_2^{-1} u(k_{n_1} \ell_2, r_2) Y_{\ell_2 m_2}(\Omega_2) \ , \tag{5}$$

$$\phi(n_1 \ell_1 m_1, \mathbf{r}_1) = r_1^{-1} P(n_1 \ell_1, r_1) Y_{\ell_1 m_1}(\Omega_1) \ . \tag{6}$$

Here $\phi(n_1 \ell_1 m_1, \mathbf{r}_1)$ is the hydrogen atom wave function with radial part $r_1^{-1} P(n_1 \ell_1, r_1)$ and angular part $Y_{\ell_1 m_1}(\Omega_1)$ and quantum numbers $n \ell_1 m_1$; $r_2^{-1} u(k_{n_1} \ell_2, r_2)$ is the radial part and $Y_{\ell_2 m_2}(\Omega_2)$ is the angular part of the free electron wave function with quantum numbers $k_{n_1} \ell_2 m_2$. The relation between the wave number k_{n_1} and n_1 is given by

$$k_{n_1}^2 = 2\left(E + \frac{1}{2n_1^2}\right) \ . \tag{7}$$

Finally the constants $C^{\ell_1 \ell_2 L}_{m_1 m_2 M} = (\ell_1 \ell_2 m_1 m_2 | LM)$, with M representing the total magnetic quantum number, are vector coupling coefficients which make the linear combination of the products of the one electron wave function in Equation 5 the eigenfunction of L. In the problem under consideration, $n_1 = 1, 2$; $\ell_1 = 0, 1$; $\ell_2 = |L-\ell_1|, \cdots, |L+\ell_1|$; $m_1 = -\ell_1, \cdots, \ell_1$; and $m_2 = -\ell_2, \cdots, \ell_2$. To make the total wave function symmetric for antiparallel spins or antisymmetric for parallel spins, the operator P_{12} interchanges $\mathbf{r}_1$ and $\mathbf{r}_2$ while β is +1 for the first case and is -1 for the second.

By taking L perpendicular to the z-axis, $M = 0$ and $m_2 = -m_1$. Equation 5 can then be written

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = (1+\beta P_{12}) \sum_{n_1 \ell_1 \ell_2} \sum_{m_1} C^{\ell_1 \ell_2 L}_{m_1 -m_1 0} \phi(n_1 \ell_1 m_1, \mathbf{r}_1)$$

$$\times\ r_2^{-1} u(k_{n_1} \ell_2, r_2) Y_{\ell_2 m_2}(\Omega_2) \ . \tag{8}$$

In order that $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ closely approximates the exact wave function, we minimize the expectation value of the energy operator with respect to the radial parts of the free electron wave functions,

$$\delta \int \psi_L^*(\mathbf{r}_1, \mathbf{r}_2) [H-E] \psi_L(\mathbf{r}_1, \mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2 = 0 \ . \tag{9}$$

It has been shown by Kohn (Reference 7) that the differences between the scattering amplitudes obtained from these equations and the exact scattering amplitudes are quadratic in the difference between $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ and the exact wave function. When the variation is carried out inside the integral, we obtain

$$\sum_{m_1} C^{\ell_1 \ell_2 L}_{m_1 -m_1 0} \int \phi^*(n_1 \ell_1 m_1, \mathbf{r}_1)\, Y^*_{\ell_2 m_2}(\Omega_2)\, [H - E]\, \psi_L(\mathbf{r}_1, \mathbf{r}_2)\, d^3\mathbf{r}_1\, d\Omega_2 = 0 . \tag{10}$$

By means of Equations 2 and 8, the Schroedinger equation for the hydrogen atom,

$$\left[\nabla_1^2 + \frac{2}{r_1}\right] \phi(n_1 \ell_1 m_1, \mathbf{r}_1) = \frac{1}{n_1^2}\, \phi(n_1 \ell_1 m_1, \mathbf{r}_1) , \tag{11}$$

and Equation 7, Equation 10 reduces to

$$\sum_{m_1} \sum_{n_1' \ell_1' \ell_2'} \sum_{m_1'} C^{\ell_1 \ell_2 L}_{m_1 -m_1 0}\, C^{\ell_1' \ell_2' L}_{m_1' -m_1' 0} \int \phi^*(n_1 \ell_1 m_1, \mathbf{r}_1)\, Y^*_{\ell_2 m_2}(\Omega_2)\, (1 + \beta P_{12})$$

$$\times \left[\nabla^2_{r_2} - \frac{\ell_2' (\ell_2' + 1)}{r_2^2} + k^2_{n_1'} + 2\left(\frac{1}{r_2} - \frac{1}{r_{12}}\right)\right] \phi(n_1' \ell_1' m_1', \mathbf{r}_1)$$

$$\times\, r_2^{-1}\, u\left(k_{n_1'} \ell_2', r_2\right) Y_{\ell_2' m_2'}(\Omega_2)\, d^3\mathbf{r}_1\, d\Omega_2 = 0 , \tag{12}$$

where $\nabla^2_{r_2}$ is the radial part of ∇_2^2. By orthogonality of the hydrogen atom and spherical harmonics wave functions, the relation (Reference 8)

$$\sum_{m_1} \left[C^{\ell_1 \ell_2 L}_{m_1 -m_1 0}\right]^2 = 1 , \tag{13}$$

the integration by parts of the exchange terms, and the relation*

$$C^{\ell_2 \ell_1 L}_{-m_1 m_1 0} = (-)^{L - \ell_1 - \ell_2}\, C^{\ell_1 \ell_2 L}_{m_1 -m_1 0} , \tag{14}$$

*Reference 8, Equation 3.16b.

Equation 12 leads to

$$\left[\nabla_{r_2}^2 - \frac{\ell_2(\ell_2+1)}{r_2^2} + k_{n_1}^2 + \frac{2}{r_2}\right]\frac{u(k_{n_1}\ell_2, r_2)}{r_2} - 2\sum_{m_1}\sum_{n_1'\ell_1'\ell_2'}\sum_{m_1'} C^{\ell_1\ell_2 L}_{m_1 -m_1 0}\, C^{\ell_1'\ell_2' L}_{m_1' -m_1' 0}$$

$$\int \frac{\phi^*(n_1\ell_1 m_1, \mathbf{r}_1)\, Y^*_{\ell_2 m_2}(\Omega_2)}{r_{12}} \times \left[\phi(n_1'\ell_1' m_1', \mathbf{r}_1)\frac{u(k_{n_1}'\ell_2', r_2)}{r_2} Y_{\ell_2' m_2'}(\Omega_2)\right.$$

$$\left. + \beta\phi(n_1'\ell_1' m_1', \mathbf{r}_2) \times \frac{u(k_{n_1}'\ell_2', r_1)}{r_1} Y_{\ell_2' m_2'}(\Omega_1)\right] d^3\mathbf{r}_1\, d\Omega_2$$

$$+ \beta \sum_{n_1'\ell_1'\ell_2'} (-)^{L-\ell_1-\ell_2}\,\delta(\ell_1'\ell_2', \ell_2\ell_1)\left(\frac{1}{n_1^2} + k^2_{n_1'}\right)$$

$$\int_0^\infty P(n_1\ell_1, r_1)\, r_2^{-1} P(n_1'\ell_1', r_2) \times u(k_{n_1'}\ell_2', r_1)\, dr_1 = 0 . \quad (15)$$

If $1/r_{12}$ is expanded in terms of the Legendre polynomials and use is made of the addition theorem,* we obtain

$$\frac{1}{r_{12}} = \sum_{\lambda=0}^{\infty} \frac{r_<^\lambda}{r_>^{\lambda+1}} P_\lambda(\cos\theta_{12})$$

$$= \sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{+\lambda} \frac{4\pi}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}} Y_{\lambda\mu}(\Omega_1)\, Y^*_{\lambda\mu}(\Omega_2) . \quad (16)$$

In this expression θ_{12} is the angle between the position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ at the origin, and $r_<$ is the smaller and $r_>$ is the larger of $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$. We also introduce

$$\mathcal{Y}_\lambda(n\ell n'\ell', r_2) = r_2^{-(\lambda+1)}\int_0^{r_2} P(n\ell, r_1)\, P(n'\ell', r_1)\, r_1^\lambda\, dr_1$$

$$+ r_2^\lambda \int_{r_2}^\infty P(n\ell, r_1)\, P(n'\ell', r_1)\, r_1^{-(\lambda+1)}\, dr_1 . \quad (17)$$

*Reference 8, Equation 4.28.

Then it follows that

$$\int_0^\infty \frac{P(n\ell,\, r_1)\, P(n'\ell',\, r_1)}{r_{12}}\, dr_1 = \sum_{\lambda=0}^{\infty} \sum_{m=-\lambda}^{+\lambda} Y_{\lambda\mu}(\Omega_1)\, Y^*_{\lambda\mu}(\Omega_2)\, \mathcal{Y}_\lambda\left(n\ell\; n'\ell',\, r_2\right) . \tag{18}$$

By means of Equation 18, the relation*

$$\int Y^*_{\ell_3 m_3}\, Y_{\ell_2 m_2}\, Y_{\ell_1 m_1}\, d\Omega = \left[\frac{(2\ell_1+1)\,(2\ell_2+1)}{4\pi\,(2\ell_3+1)}\right]^{1/2} C^{\ell_1\ell_2\ell_3}_{m_1 m_2 m_3}\, C^{\ell_1\ell_2\ell_3}_{000} , \tag{19}$$

and the definition

$$\left(n\ell | k_{n_1} \ell'\right) = \int_0^\infty P(n\ell,\, r)\, u\left(k_{n_1} \ell',\, r\right) dr , \tag{20}$$

Equation 15 when multiplied by r_2 gives

$$\left[\frac{d^2}{dr_2^{\,2}} - \frac{\ell_2(\ell_2+1)}{r_2^{\,2}} + k_{n_1}^2 + \frac{2}{r_2}\right] u\left(k_{n_1} \ell_2,\, r_2\right)$$

$$- 2\left(\frac{2\ell_2+1}{2\ell_1+1}\right)^{1/2} \sum_{n_1'\ell_1'\ell_2'} \sum_{m_1 m_1'} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{+\lambda} C^{\ell_1\ell_2 L}_{m_1 -m_1 0}\, C^{\ell_1'\ell_2' L}_{m_1' -m_1' 0}$$

$$\times \left\{\left(\frac{2\ell_1'+1}{2\ell_2'+1}\right)^{1/2} C^{\lambda\ell_1'\ell_1}_{\mu m_1' m_1}\, C^{\lambda\ell_1'\ell_1}_{000}\, C^{\lambda\ell_2\ell_2'}_{\mu m_2 m_2'}\, C^{\lambda\ell_2\ell_2'}_{000}\, \mathcal{Y}_\lambda\left(n_1 \ell_1\, n_1' \ell_1',\, r_2\right) u\left(k_{n_1'} \ell_2',\, r_2\right)\right.$$

$$\left. + \beta\left(\frac{2\ell_2'+1}{2\ell_1'+1}\right)^{1/2} C^{\lambda\ell_2'\ell_1}_{\mu m_2' m_1}\, C^{\lambda\ell_2'\ell_1}_{000}\, C^{\lambda\ell_2\ell_1'}_{\mu m_2 m_1'}\, C^{\lambda\ell_2\ell_1'}_{000}\, P\left(n_1'\ell_1',\, r_2\right) \mathcal{Y}_\lambda\left(n_1 \ell_1\, k_{n_1'} \ell_2',\, r_2\right)\right\}$$

$$+ \beta \sum_{n_1'\ell_1'\ell_2'} (-)^{L-\ell_1-\ell_2}\, \delta\left(\ell_1'\ell_2',\, \ell_2\ell_1\right) \left(\frac{1}{n_1^2} + k_{n_1'}^2\right) P\left(n_1'\ell_1',\, r_2\right) \left(n_1 \ell_1 | k_{n_1'} \ell_2'\right) = 0 . \tag{21}$$

In the exchange integrals above we have defined $P\left(k_{n_1} \ell_2,\, r\right)$ as $u\left(k_{n_1} \ell_2,\, r\right)$.

---

*Reference 8, Equation 4.34.

The vectorial equations

$$L = \ell_1 + \ell_2 , \tag{22}$$

where L is constant but ℓ_1 and ℓ_2 take the values given before, can be divided into two groups, one with $L - \ell_1 - \ell_2$ even and the other with $L - \ell_1 - \ell_2$ odd. Since the total spatial wave function has the parity of $\ell_1 + \ell_2$, in the first group the wave function has the parity of L and in the second a parity opposite to L. By conservation of parity we have two distinct groups of interactions. In this problem, where 1s, 2s, and 2p states of atomic hydrogen are taken into account, it is easy to see that, when $L - \ell_1 - \ell_2$ is even, the set of quantum numbers $k_{n_1} \ell_2$ has four values: one for each of the 1s and 2s states, and two for the 2p state. When $L - \ell_1 - \ell_2$ is odd, $k_{n_1} \ell_2$ has one value which corresponds to the elastic scattering of electrons by the 2p state of the hydrogen atom. Equation 21 is evaluated for these cases, and the resulting differential equations are listed in Appendix A. In evaluating Equation 21, it should be noted that the $C^{\ell_1 \ell_2 \ell_3}_{m_1 m_2 m_3}$ coefficients are subject to the condition that $\ell_1 \ell_2 \ell_3$ form a closed triangle and $m_3 = m_1 + m_2$.* This limits the summation over λ and μ considerably to few terms only. Summation over m_1, m_1', λ, and μ is carried out using the numerical values of the C coefficients given by Condon and Shortley (Reference 9).

Percival and Seaton (Reference 3) have derived the same differential equations for the scattering of free electrons by atomic s, p, and d electrons in the hydrogen atom using the theory of irreducible tensor operators to evaluate the interaction terms between the two electrons in the differential equations. The calculation becomes considerably simpler in this way. The results of the two methods are identical.

In the rest of the paper, except the section on page 14, we discuss the solutions to the four coupled differential equations given in Appendix A and which arise when $L - \ell_1 - \ell_2$ is even. The single differential equations for $L - \ell_1 - \ell_2$ odd are derived in the excepted section (page 14). Its numerical integration can be treated as a special case of the four coupled differential equations.

When the integrals representing the direct potentials in the four differential equations are evaluated and some change is made in the limits of the exchange potential integrals, these equations can be written in the following matrix form:

$$\left[\frac{d^2}{dr^2} + k_n^2 - \frac{l_n (l_n + 1)}{r^2} \right] \mathbf{u}(k_n l_n, r) = 2\mathbf{V}\mathbf{u}(k_n l_n, r) . \tag{23}$$

The four components of $\mathbf{u}$ are the four radial functions of the free electron. $\mathbf{V}$ is a 4x4 symmetric matrix that is the sum of three matrices,

$$\left. \begin{aligned} V_{ij} &= D_{ij} + E_{ij} , \\ E_{ij} &= F_{ij} + \sum_{\nu=1}^{\sigma} g_{ij}^{\nu} \int_0^{\infty} h_{ij}^{\nu} \, dr , \end{aligned} \right\} \tag{24}$$

*Reference 8, Equation 3.14.

where D_{ij} is the direct potential, E_{ij} is the exchange potential, and where both are functions of r. The matrix E_{ij} contains in addition integrals with respect to r, and for the purpose of numerical integration it can be written as the sum of two matrices. The explicit forms of D_{ij}, F_{ij}, g_{ij}^{ν}, and h_{ij}^{ν} are given in Appendix B. The value of σ is 2 for $i = j = 3$ and $i = j = 4$, and is 1 for all other values of i and j. It is understood that for the exchange terms the components of $\mathbf{u}$ on the right-hand side of Equation 23 are inside the integrals of the exchange terms.

Derivation of the Transmission Matrix from Solutions of the Differential Equations

The method is similar to that used by Bransden and McKee (Reference 10), and by Marriot (Reference 1). Equation 23 constitutes a set of four coupled second-order differential equations. Three components of $\mathbf{u}$ can be eliminated from these equations, resulting in an 8^{th} order differential equation for the remaining component. Therefore there are eight sets of solutions to Equation 23. However, only half of these solutions are regular at the origin. Each of the four regular solutions corresponds to a definite vector $\mathbf{u}$. The four vectors can properly be represented by a 4x4 matrix u_{nj}, $n, j = 1, 2, 3, 4$, where n corresponds to the particular component and j correreponds to the particular solution of $\mathbf{u}$. The four solutions are carried out numerically in the next section.

From the explicit form of $\mathbf{V}$ it can be seen that $\mathbf{V}$ vanishes at infinity. The asymptotic solution of $\mathbf{u}$ as given by Equation 23 is therefore

$$u_{nj}(r) \approx a_{nj} \sin\left(k_n r - \frac{l_n \pi}{2} + \delta_{nj}\right) \quad (n, j = 1, 2, 3, 4) \, , \tag{25}$$

where a_{nj} is the amplitude and δ_{nj} is the phase shift of the j^{th} solution of the n^{th} component of $\mathbf{u}$.

Corresponding to the four components of $\mathbf{u}$, there are 4 channels open to the reaction. If the incident wave is in the m^{th} channel ($m = 1, 2, 3, 4$), the traveling wave in the n^{th} channel will be given by

$$u_n(r) \approx \exp\left[-i\left(k_n r - \frac{1}{2} l_n \pi\right)\right] \delta(m, n) - S_{mn} \exp\left[i\left(k_n r - \frac{1}{2} l_n \pi\right)\right] \quad (n = 1, 2, 3, 4) \, . \tag{26}$$

The constants S_{mn} are the amplitudes of the scattered waves. Since Equation 26 is also the asymptotic solution of Equation 23, they must be equal to linear combinations of Equation 25. If we call the coefficients of the linear combinations P_j, we must have

$$\sum_{j=1}^{4} P_j a_{nj} \sin\left(k_n r - \frac{l_n \pi}{2} + \delta_{nj}\right) =$$

$$(k_n)^{-1/2} \left\{\exp\left[-i\left(k_n r - \frac{1}{2} l_n \pi\right)\right] \delta(m, n) - S_{mn} \exp\left[i\left(k_n r - \frac{1}{2} l_n \pi\right)\right]\right\}$$

$$(n, m = 1, 2, 3, 4) \, . \tag{27}$$

On the right-hand side, we have used the normalization of Blatt and Weisskopf (Reference 11). If we equate the coefficients of $\exp\left[-i\left(k_n r - 1/2\ l_n \pi\right)\right]$ and $\exp\left[i\left(k_n r - 1/2\ l_n \pi\right)\right]$ in Equation 27, we obtain

$$\left.\begin{aligned} \sum_{j=1}^{4} P_j\, a_{nj} \exp - \left[i\, \delta_{nj}\right] &= \frac{-2i}{\sqrt{k_n}}\, \delta(m, n)\ , \\ \sum_{j=1}^{4} P_j\, a_{nj} \exp \left[i\, \delta_{nj}\right] &= \frac{-2i}{\sqrt{k_n}}\, S_{mn}\ . \end{aligned}\right\} \tag{28}$$

Separation of Equations 28 into real and imaginary parts gives

$$\left.\begin{aligned} \sum_{j=1}^{4} \left[\left(\Re P_j\right) \sin \delta_{nj} - \left(\Im P_j\right) \cos \delta_{nj}\right] a_{nj} &= \frac{2}{\sqrt{k_n}}\, \delta(m, n)\ , \\ \sum_{j=1}^{4} \left[\left(\Re P_j\right) \cos \delta_{nj} + \left(\Im P_j\right) \sin \delta_{nj}\right] a_{nj} &= 0\ , \\ \sum_{j=1}^{4} \left[\left(\Re P_j\right) \sin \delta_{nj} + \left(\Im P_j\right) \cos \delta_{nj}\right] a_{nj} &= \frac{-2}{\sqrt{k_n}}\, \Re S_{mn}\ , \\ \sum_{j=1}^{4} \left[\left(\Re P_j\right) \cos \delta_{nj} - \left(\Im P_j\right) \sin \delta_{nj}\right] a_{nj} &= \frac{2}{\sqrt{k_n}}\, \Im S_{mn}\ . \end{aligned}\right\} \tag{29}$$

In the above $\Re$ or $\Im$ represent the real or the imaginary part of the quantity that follows them. Equations 29 are a set of 16 linear equations for 16 unknowns $\Re P_j$, $\Im P_j$, $\Re S_{mn}$ and $\Im S_{mn}$. Once these unknowns are found,* the magnitude of S_{mn} will be given by

$$\left|S_{mn}\right|^2 = \left(\Re S_{mn}\right)^2 + \left(\Im S_{mn}\right)^2\ . \tag{30}$$

*Equations 29 with their present form and without further simplifications are solvable by the computer.

The cross section is obtained by asymptotic expansion in spherical harmonics of the incident plane wave*

$$\exp[ikz] \approx \frac{\pi^{1/2}}{kr} \sum_{l=0}^{\infty} (2l+1)^{1/2}\, i^{l+1} \left\{ \exp\left[-i\left(kr - \frac{1}{2}\, l\pi\right)\right] - \exp\left[i\left(kr - \frac{1}{2}\, l\pi\right)\right] \right\} Y_{l,0} \quad . \tag{31}$$

The magnitude of the ingoing wave on the right-hand side of Equation 27 for $n = m$ is $\left[k_m/\pi\left(2l_m+1\right)\right]^{1/2}$ times the magnitude of the partial wave of the expansion of $r \exp\left[ik_m z\right]$. The plane wave has a flux of v which, in atomic units, is equal to k. The ingoing flux of the right-hand side of Equation 27 is therefore $k_m^2/\left[\pi\left(2l_m+1\right)\right]$. The outgoing flux in the channel $n \neq m$ is $|S_{mn}|^2$. The cross section is obtained when we average the ratio of the outgoing flux to the ingoing flux over the initial states and sum over the final states. For a particular spin state of the two electrons, unpolarized electron beam, and unoriented atoms, the multiplicity of the initial states is $\left(2l_1+1\right)\left(2l_2+1\right)$, where l_1 and l_2 are the angular momentum of the bound and free electrons. For a polarized beam, $m_2 = 0$, where m_2 is the magnetic quantum number of the free electron. Then $m_1 = M$, where m_1 and M are the bound electron and the total magnetic quantum numbers. Since M is constant, there is only one initial state for a polarized beam. The multiplicity of the final states is $2L+1$, where L is the total orbital angular momentum. Since $\ell_m = \ell_2$, the cross section for $m \neq n$ is

$$Q_{mn} = \frac{\pi\left(2L+1\right)}{k_m^2\left(2l_1+1\right)} \left|S_{mn}\right|^2 \quad (m \neq n) \quad . \tag{32}$$

The outgoing partial wave in the incident channel m consists of the scattered wave plus the outgoing wave given in the expansion of the plane wave. Then, according to Equation 27 for $n = m$, the magnitude of the amplitude of the scattered wave is $\left|1 - S_{mn}\right|$. The elastic scattering cross section is therefore given by

$$Q_{mm} = \frac{\pi\left(2L+1\right)}{k_m^2\left(2l_1+1\right)} \left|1 - S_{mm}\right|^2 \quad . \tag{33}$$

If we define a matrix T by the relation

$$T = 1 - S \ , \tag{34}$$

*Reference 11, Ch. VIII, Equation 2.7.

Equations 32 and 33 can then be combined into a single equation,

$$Q_{mn} = \frac{\pi(2L+1)}{k_m^2(2l_1+1)} |T_{mn}|^2 . \tag{35}$$

T_{mn} is the transmitted amplitude in the n^{th} channel due to an incident wave in the m^{th} channel. The elements of T_{mn} constitute the transmission matrix.

The matrix S has two properties that are useful as tests on the accuracy of numerical integration. From Equation 26 it can be seen that S transforms the ingoing wave into the outgoing waves. The continuity of the electronic current requires that S be a unitary matrix

$$\sum_{n=1}^{4} |S_{mn}|^2 = 1 \quad (m = 1, 2, 3, 4) . \tag{36}$$

Furthermore, since the Hamiltonian is Hermetian, S must be symmetric (Reference 11):

$$S_{mn} = S_{nm} . \tag{37}$$

Equations 36 and 37 are used as tests on the accuracy of numerical integration.

A Useful Relation

A relation based on the symmetry of the interaction potentials, which serves as another test on the accuracy of the solutions, can be derived. The l^{th} and the k^{th} solutions of the i^{th} component of **u** by Equation 23 are given by

$$\left.\begin{aligned} \left[\frac{d^2}{dr^2} + k_i^2 - l_i \frac{(l_i+1)}{r^2}\right] u_{il} &= \sum_j V_{ij} u_{jl} , \\ \left[\frac{d^2}{dr^2} + k_i^2 - l_i \frac{(l_i+1)}{r^2}\right] u_{ik} &= \sum_j V_{ij} u_{jk} . \end{aligned}\right\} \tag{38}$$

Multiplying the first by u_{ik} and the second by u_{il}, subtracting the two expressions, and summing over i gives

$$\sum_i \left[u_{ik} \frac{d^2}{dr^2} u_{il} - u_{il} \frac{d^2}{dr^2} u_{ik}\right] = \sum_{i,j} V_{ij} \left[u_{ik} u_{jl} - u_{il} u_{jk}\right] . \tag{39}$$

Since $V_{ij} = V_{ji}$, the interchange of the summation indices changes the sign on the right-hand side of the equation; the right-hand side must therefore be zero. Integrating the left-hand side from zero to infinity, we obtain

$$\sum_i \int_0^\infty \left[u_{ik} \frac{d^2}{dr^2} u_{il} - u_{il} \frac{d^2}{dr^2} u_{ik}\right] dr = 0 . \tag{40}$$

Integrating the above equation by parts, and applying Equation 25, we obtain

$$\sum_{i=1}^{4} k_i \, a_{ik} \, a_{il} \sin\left(\delta_{ik} - \delta_{il}\right) = 0 \qquad (k, l = 1, 2, 3, 4, k \neq l) . \tag{41}$$

Although the terms containing the exchange potentials do not cancel out on the right-hand side of Equation 39, the cancellation does take place after the integration is carried out in Equation 40.

Transmission Matrix According to Born Approximation

The Born approximation consists of neglecting the exchange potential terms appearing in the V matrix of Equation 23, and also of neglecting all the direct potential terms in this matrix except those terms that connect the incident channel to all other channels (Reference 12). Equation 23, when the incident wave is in the m^{th} channel, reduces to

$$\left[\frac{d^2}{dr^2} + k_n^2 - \frac{l_n \left(l_n + 1\right)}{r^2}\right] u_n = 2 D_{nm} u_m \quad (n = 1, 2, 3, 4) ; \tag{42}$$

u_m and u_n are given asymptotically by

$$u_m \approx k_m^{-1/2} \sin\left(k_m r - l_m \frac{\pi}{2}\right) , \tag{43}$$

$$u_n \approx k_n^{-1/2} B_{nm} \cos\left(k_n r - l_n \frac{\pi}{2}\right) . \tag{44}$$

We have chosen the constants of proportionality of u_m and u_n such that B_{nm} is the Born approximation of the reactance matrix R (Reference 13).* Equation 43 shows that u_m must have the following form (Reference 14):

$$u_m = k_m^{1/2} \, r \, j_{l_m}\left(k_m r\right) , \tag{45}$$

*Also Reference 11, Ch. X, Sec. 4.

where $j_{l_m}(k_m r)$ are spherical Bessel functions. Furthermore, if y_n represents the homogenous solution of Equation 42, it must have the following forms:

$$y_n = a_n k_n r \, j_{l_n}(k_n r) \ , \tag{46}$$

$$y_n \approx a_n \sin\left(k_n r - l_n \frac{\pi}{2}\right) , \tag{47}$$

with a_n some unknown constant. Multiplying Equation 42 on the left by y_n and integrating the result from zero to infinity, we obtain by partial integration

$$2\int_0^\infty y_n D_{nm} u_m \, dr = \int_0^\infty y_n \left[\frac{d^2}{dr^2} + k_n^2 - \frac{l_n(l_n+1)}{r^2}\right] u_n \, dr$$

$$= \left[y_n \frac{d}{dr} u_n - u_n \frac{d}{dr} y_n\right]_0^\infty$$

$$= -k_n^{1/2} a_n B_{nm} \ .$$

The last equality has been obtained by noticing that y_n and u_n vanish at the origin, and by using their asymptotic forms as given by Equations 44 and 47. We therefore have

$$B_{nm} = -2(k_n k_m)^{1/2} \int_0^\infty j_{l_n}(k_n r) \, D_{nm} \, j_{l_m}(k_m r) \, r^2 \, dr \ . \tag{48}$$

This is identical to the expression given for $\mathbf{B}$ by Seaton.*

The transmission and the reactance matrices are related by $\mathbf{T} = -2i\mathbf{R}/(1 - i\mathbf{R})$. Since in the Born approximation $\mathbf{R} = \mathbf{B} \ll 1$, the transmission matrix according to the Born approximation is given by

$$T^B_{nm} = 4i\,(k_n k_m)^{1/2} \int_0^\infty j_{\ell_n}(k_n r) \, D_{nm} \, j_{\ell_m}(k_m r) \, r^2 \, dr \ . \tag{49}$$

Substitution of Equation 49 into 35 would give the cross section according to the Born approximation. It should be noted that the symmetry of $\mathbf{T}$ insures Equation 37 to be satisfied while Equation 36 is no longer satisfied.

*Reference 13, Equation 3.10.

Elastic Scattering of Electrons by the 2p States of the Hydrogen Atom

The angular momentum of the free electron l_2 in the 2p channel has the values $L - 1, L, L + 1$, where L is the total angular momentum of the system. The first and the last values were considered in previous sections. The case $l_2 = L$ corresponds to a wave function in the 2p channel with a parity different from all channel wave functions considered previously. It therefore corresponds to elastic scattering. The wave function in this case is given by

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = (1 + \beta P_{12}) \sum_{m_1=-1}^{+1} C^{1LL}_{m_1-m_1 0} \, \phi_{2pm_1}(\mathbf{r}_1) \frac{u(k_2 L, \mathbf{r}_2)}{\mathbf{r}_2} Y_{L-m_1}(\Omega_2) \; . \tag{50}$$

When Equation 9 is formed with this wave function, and minimized with respect to $u(k_2 L, r_2)$, treatment which led to the derivation of the four differential equations will give the following differential equation:

$$\begin{aligned} &\left[\frac{d^2}{dr^2} + k_2^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u_L(r) \\ &- \beta\left(\frac{1}{4} + k_2^2\right) \delta(L, 1)\, r\, R_{21}(r) \left(2p \middle| k_2 L\right) \\ &+ 2\left[y_0(2p\,2p, r) - \frac{1}{5} y_2(2p\,2p, r)\right] u_L(r) \\ &+ 2\beta r R_{21}(r) \left[-\frac{3y_{L-1}(2p\,k_2 L, r)}{(2L+1)(2L-1)} + \frac{3y_{L+1}(2p\,k_2 L, r)}{(2L+1)(2L+3)}\right] = 0 \; , \end{aligned} \tag{51}$$

The asymptotic solution of this equation is given by

$$u_L \approx a_L \sin\left(k_2 r - L\pi/2 + \delta_L\right) \; . \tag{52}$$

If the scattering amplitude is designated by T_{55}, it can be shown from the section on page 8 that for a particular L

$$T_{55} = 1 - \exp 2i\delta = -2i \exp(i\delta) \sin\delta \; , \tag{53}$$

where for simplicity we have suppressed the subscript L. The cross section, according to Equation 35, is given by

$$Q_{55} = \frac{4\pi(2L+1)}{3k_2^2} \sin^2\delta \; . \tag{54}$$

The total elastic scattering cross section by the 2p states is the sum of this cross section and the cross section corresponding to $l_2 = L - 1$ and $l_2 = L + 1$ (which were considered previously).

The Born amplitude, Equation 48, in this case is given by

$$B_{55} = -2k_2 \int_0^\infty j_L(k_2 r)\, D_{55}\, j_L(k_2 r)\, r^2\, dr \,, \tag{55}$$

where, by Equation 51,

$$D_{55} = -\frac{1}{r} + y_0\,(2p\,2p,\, r) - \frac{1}{5}\, y_2\,(2p\,2p,\, r) \,. \tag{56}$$

NUMERICAL INTERGRATION

Decomposition of the Differential Equations

If it were not for the definite integrals appearing in the potential matrix $\mathbf{v}$, the set of the four coupled differential equations (23) could be integrated by any standard technique. The presence of these unknown constants whose integrand involves the unknown functions makes it necessary to solve these equations by iteration or by transformation of $\mathbf{u}$ into other vectors, whose differential equations do not contain definite integrals. Since the terms containing definite integrals are small as compared with the direct potentials, the iteration method can be used by assuming that the values of these integrals are zero. The differential equations are then integrated, the values of the definite integrals that are subsequently obtained are substituted in the differential equations, and the integration is repeated. The process is repeated until sufficiently consistent values of these integrals are obtained. This method is useful if the convergences of the constants are fast enough, and the cross section is not very sensitive to the values of these constants.

In the second method, the transformation of $\mathbf{u}$ fixes the values of the constants and thus avoids iteration, whereby the computation is reduced considerably. The description of the method will be given here (Reference 15).*

By making use of Equations 24, Equation 23 can be written

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i\,(l_i + 1)}{r^2}\right] u_i = 2 \sum_{j=1}^{4} \left[\left(D_{ij} + F_{ij}\right) u_j + \sum_{\mu=1}^{\sigma} g_{ij}^{\mu}\, C_{ij}^{\mu}\right] , \tag{57}$$

*Also, Reference 1. This description differs from the description of Reference 15 and the present paper. In Reference 1, v_i in Equation 61 is set to 0; this makes $B_{ij}^{\mu} = 0$. Equations 62 then reduce to a set of homogeneous equations whose determinant must be 0. Since the amplitude of any of the four components of $\mathbf{u}$ can be left arbitrary, one of the C_{kl}^{ν} is set equal to 1 and the rest of the constants are found subsequently.

where

$$C_{ij}^{\mu} = \int_0^{\infty} h_{ij}^{\mu}(r) u_j(r) dr \ . \tag{58}$$

We introduce the functions v_i and u_i^{kl} that are solutions of the following differential equations:

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2}\right] v_i = 2 \sum_{j=1}^{4} \left[D_{ij} + F_{ij}\right] v_j \ , \tag{59}$$

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2}\right] u_i^{kl} = 2 \sum_{j=1}^{4} \left[D_{ij} + F_{ij}\right] u_j^{kl} + 2\delta(i,k) g_{kl}^{\nu} \ . \tag{60}$$

Then u_i is given by the following expression:

$$u_i = v_i + \sum_{k=1}^{4} \sum_{l=1}^{4} \sum_{\nu=1}^{\sigma} C_{kl}^{\nu} u_i^{kl} \ . \tag{61}$$

Equation 61 can be verified by multiplying Equation 60 by C_{kl}^{ν}; summing over k, l, and ν; and adding to Equation 59—whereupon Equation 57 results. Substitution of Equation 61 in Equation 58 gives

$$\sum_{k=1}^{4} \sum_{l=1}^{4} \sum_{\nu=1}^{\sigma} \left[\delta(ij\mu, kl\nu) - A_{ij}^{\mu kl}\right] C_{kl}^{\nu} = B_{ij}^{\mu}$$

$$(i, j = 1, 2, 3, 4;\ \mu = 1, 2 \text{ for } i = j = 3 \text{ and } i = j = 4;\ \mu = 1 \text{ otherwise}) \ , \tag{62}$$

where $A_{ij}^{\mu kl}$ and B_{ij}^{μ} are defined by

$$\left.\begin{aligned} A_{ij}^{\mu kl} &= \int_0^{\infty} h_{ij}^{\mu} u_j^{kl} dr \ , \\ B_{ij}^{\mu} &= \int_0^{\infty} h_{ij}^{\mu} v_j \, dr \ . \end{aligned}\right\} \tag{63}$$

The numerical integration is carried out by integrating Equations 59 and 60 by any standard method, calculating $A_{ij}^{\mu kl}$ and B_{ij}^{μ} by Equations 63 and, finally, solving the system of 18 algebraic equations given by Equation 62 to find C_{kl}^{ν}. With the known values of these constants the integration of Equation 57 is straightforward.

The determinant of Equation 62 becomes singular for $L = 0$ and 1. This is shown in Appendix C. To remove the singularity, some of the C_{kl}^{ν} are chosen arbitrarily, and the rest of the C_{kl}^{ν} are found in terms of the chosen ones.

Solution at the Origin

In order that the four solutions of u be independent of each other, we must have

$$\sum_{j=1}^{4} C_j u_{ij} \neq 0 \quad (i = 1, 2, 3, 4) , \tag{64}$$

where C_j are some constants. A necessary condition for this to be satisfied is that the determinant of Equation 64 be nonzero:

$$||u_{ij}|| \neq 0 . \tag{65}$$

It is not difficult to see that this also is a sufficient condition. At the origin the solution u_{ij} can be expressed as power series in r,

$$u_{ij} = \sum_{\nu=0}^{\infty} a_{ij}^{\nu} r^{s_i+\nu} , \tag{66}$$

where a_{ij}^{ν} are the coefficients of expansion, and s_i are given integers for each component of u and are fixed by the behavior of Equation 23 at the origin. We can satisfy Equation 65 at the origin by having

$$||a_{ij}^{0}|| \neq 0 . \tag{67}$$

By choosing suitable values of a_{ij}^{0}, subject to the restriction of Equation 67, four independent solutions are obtained.

Solution at Large r

With given initial values, the solution of Equation 23 can be extended from origin to any desired value of r. To obtain the asymptotic amplitudes and the phase shifts, the presence of the centrifugal and long-range potentials makes it necessary to extend the solutions to infinity. This is undesirable because of the time consumption on the computer, and the accumulated error due to the long-range integration. Seaton (Reference 13) has solved the problem of r^{-2} long-range potentials occurring in the off-diagonal terms of the potential matrix V by diagonalizing the asymptotic form of the differential Equation 23 and the corresponding S-matrix. By an inverse transformation the elements of the original S-matrix are found.

Instead, we develop here a perturbation theory which is based on the method described by Mott and Massey (Reference 16). The error in the resulting solution is inversely proportional to the square of the distance from the origin.

Equation 23 for large distances of r can be written

$$\left[\frac{d^2}{dr^2} + k_n^2\right] \mathbf{u}\left(k_n\, l_n,\, r\right) = 2\mathbf{U}\mathbf{u}\left(k_n\, l_n,\, r\right) , \tag{68}$$

where $\mathbf{U}$ is the sum of the centrifugal potential matrix and the asymptotic form of the $\mathbf{V}$ matrix. The elements of $\mathbf{U}$ are given in Appendix D. A component of Equation 68 is of the following form:

$$\left.\begin{aligned} \left[\frac{d^2}{dr^2} + k^2\right] u(r) &= g(r) , \\ g(r) &<< k^2 u(r) \quad \left(g(r) \to 0 \text{ as } r \to \infty\right) . \end{aligned}\right\} \tag{69}$$

The perturbation theory is applied between some large distance R and infinity. Suppose u vanishes at R; then we have the following boundary condition:

$$u(R) = 0 . \tag{70}$$

If we represent the solution of the homogenous equation by $y(r)$, at infinity, we must have

$$\left.\begin{aligned} y(r) &= a \sin(kr - kR) , \\ u(r) &= (a + \Delta a) \sin(kr - kR + \eta) , \end{aligned}\right\} \tag{71}$$

where a is the amplitude of $u(r)$ if $g(r)$ were identically zero and ΔA and η are generated by $g(r)$. Since $g(r)$ is small, we can write

$$u = y(1 + \zeta) , \tag{72}$$

where ζ is a small function. Substitution of Equation 72 in Equation 69 gives

$$\frac{d}{dr}\left(y^2 \frac{d\zeta}{dr}\right) = g(r)\, y , \tag{73}$$

where, upon double integration, we obtain

$$\zeta = \int_R^r \frac{dr}{y^2} \int_R^r g(r')\, y\, dr' . \tag{74}$$

The constants of integrations are fixed by the condition (70) and the fact that $u'(R) = y'(R)$.

We now integrate Equation 74 by parts,

$$\zeta = \left[\int_R^r g(r)\, y\, dr\right]\left[\int_R^r \frac{dr}{y^2}\right] - \int_R^r g(r)\, y\, dr \int_R^r \frac{dr}{y^2} \, . \tag{75}$$

When the integration with respect to y is carried out, and the result is substituted in Equation 73, we obtain

$$u(r) = \sin(kr - kR)\left[a + \frac{1}{k}\int_R^r g(r)\cos(kr - kR)\, dr\right]$$

$$+ \cos(kr - kR)\left[-\frac{1}{k}\int_R^r g(r)\sin(kr - kR)\, dr\right] . \tag{76}$$

Comparison of the second of Equations 71 and 76 shows that

$$\left.\begin{aligned} \Delta a &= \frac{1}{k}\int_R^\infty g(r)\cos(kr - kR)\, dr \, , \\ \eta &= -\frac{1}{ak}\int_R^\infty g(r)\sin(kr - kR)\, dr \end{aligned}\right\} \tag{77}$$

to first order. The functions $g(r)$ in the four differential Equations 68 are given by

$$g_i(r) = 2\sum_j U_{ij} u_j \, . \tag{78}$$

To first order this can be written by

$$g_i(r) = 2\sum_j a_j U_{ij} \sin\left(k_j r - k_j R_j\right) \, , \tag{79}$$

where R_j is the last zero of u_j with positive slope. Substitution of this equation in Equation 77 gives

$$\left.\begin{aligned} \Delta a_i &= -\sum_j \frac{a_j}{k_i}\int^{R_i} \cos\left(k_i r - k_i R_i\right) U_{ij} \sin\left(k_j r - k_j R_j\right) dr \, , \\ \eta_i &= \sum_j \frac{a_j}{a_i k_i}\int^{R_i} \sin\left(k_i r - k_i R_i\right) U_{ij} \sin\left(k_j r - k_j R_j\right) dr \, . \end{aligned}\right\} \tag{80}$$

Δa_i and η_i can easily be calculated by substituting the values of U_{ij} from Appendix D, integrating the resulting integrals by parts, and retaining the leading terms.

The asymptotic amplitudes and phase shifts are given by

$$\left.\begin{aligned} a_i(\infty) &= a_i(R_i) + \Delta a_i , \\ \delta_i(\infty) &= \delta_i(R_i) + \eta_i + [L - \delta(i, 3) + \delta(i, 4)]\frac{\pi}{2} , \end{aligned}\right\} \tag{81}$$

where $a_i(R_i)$ and $\delta_i(R_i)$ are the amplitudes and total phase shifts calculated at R_i by the machine, and where $\delta(i, 3)$ and $\delta(i, 4)$ are the δ functions.

Details of the Numerical Integration

Milne's (Reference 17) method with variable mesh size and Simpson's* rule were used for the integration of the differential equations and evaluations of the integrals respectively. As the solution advances from the origin, the differential equations become less sensitive to the size of the increment, and the error of integration falls below certain small number ϵ. At each value of r the value of the function is found, first with the given value of the increment, and second with the value of increment divided in half. The error of integration is defined as the difference between these two solutions. When the error becomes small, the increment is doubled until a maximum value is reached. At some distance R_1 all the exchange potentials and, similarly, all the direct potentials except those representing optically allowed transitions and the $2p - 2p$ elastic scattering potential become vanishingly small (see Appendix D). At this distance the set of differential equations is replaced by the simpler set containing only these potentials. The integration is continued until some distance R_2, where the first-order solution of the rest of the range of integration is obtained by the method developed in the previous section. No attempt was made to solve any set of linear equations or any matrix equations, as these equations are solvable by the computer in their original form.

The values of the constants of the numerical integration are given below; h_i and h_f are the initial and the final increments of integration. In some exceptional cases, different values were used.

$$h_i = 1 \times 10^{-5}$$

$$h_f = 0.05$$

$$\epsilon = 1 \times 10^{-4}$$

$$R_1 = 30$$

$$R_2 = 200$$

(All quantities are in units of Bohr radius except ϵ, which is dimensionless.)

*Reference 17, Sec. 33.

RESULTS AND DISCUSSION

The differential equations (23) with the known values of the elements of the potential matrix **v** as given in Appendix B were integrated numerically by the methods described in the last section. By choosing different values for the determinant (Equation 67) different sets of independent solutions can be generated. The cross sections reported in this paper have been obtained by averaging the cross sections obtained from two independent sets of solutions. To test the accuracy of the numerical integration, we define the three quantities D_{mn}, D'_{mn}, and D''_m given by

$$D_{mn} = \frac{\left|\sum_{i=1}^{4} k_i\, a_{im}\, a_{in} \sin\left(\delta_{im} - \delta_{in}\right)\right|}{\sum_{i=1}^{4} k_i\, a_{im} a_{in} \left|\sin\left(\delta_{im} - \delta_{in}\right)\right|} \qquad (m, n = 1, 2, 3, 4,\ m \neq n) , \tag{82}$$

$$D'_{mn} = \frac{\left|S_{mn} - S_{nm}\right|}{\left|S_{mn}\right| + \left|S_{nm}\right|} \qquad (m, n = 1, 2, 3, 4,\ m \neq n) , \tag{83}$$

$$D''_m = \frac{\left|\sum_{n=1}^{4} \left|S_{mn}\right|^2 - 1\right|}{\sum_{n=1}^{4} \left|S_{mn}\right|^2 + 1} \qquad (m = 1, 2, 3, 4) . \tag{84}$$

Based on Equations 36, 37, and 41 in an exact solution of the four differential equations, the right-hand side of these equations would vanish; they can therefore be used to test the accuracy of the numerical integration. As an illustration the numerical values of D_{mn}, D'_{mn}, and D''_m for the case of 1s - 2s - 2p coupling, $\beta = +1$, $k_1 = 2.0$, and $L = 3$, are given below:

$$D_{12} = 1.4 \times 10^{-3}, \quad D_{13} = 2.6 \times 10^{-4}, \quad D_{14} = 1.3 \times 10^{-3},$$

$$D_{23} = 5.1 \times 10^{-4}, \quad D_{24} = 2.2 \times 10^{-3}, \quad D_{34} = 1.8 \times 10^{-3},$$

$$D'_{12} = 7.6 \times 10^{-4}, \quad D'_{13} = 5.1 \times 10^{-3}, \quad D'_{14} = 5.6 \times 10^{-3},$$

$$D'_{23} = 5.4 \times 10^{-3}, \quad D'_{24} = 5.7 \times 10^{-3}, \quad D'_{34} = 1.3 \times 10^{-3},$$

$$D''_1 = 1.8 \times 10^{-4}, \quad D''_2 = 7.6 \times 10^{-5}, \quad D''_3 = 2.5 \times 10^{-4}, \quad D''_4 = 4.4 \times 10^{-6} .$$

To compare the results of the numerical integration by the noniterative method we have carried out here with those of the iterative method of References 2, 4, and 5, we have provided Table 1.* The 1s → 2s excitation cross section is given by the two methods; I and II refer to the

*Author is indebted to Dr. K. Smith for sending some of the data used in Table 1.

Table 1

Comparison of the Iterative and the Noniterative Results for the Singlet ($L = 0, 1$; $k_1 = 0.9, 1.0$), $1s \rightarrow 2s$ Excitation Cross Section.*

(a) 1s - 2s coupling

k_1	L	$Q_{1s \rightarrow 2s}$		E_{max} (percent)	
		†I	II	I	II
0.90	0	0.0384	0.0375	7.1	0.72
1.00	0	0.0714	0.0725	unknown	0.53
0.90	1	0.008	0.0017	386	0.91
1.00	1	0.051	0.0583	55	0.75

(b) 1s - 2s - 2p coupling

k_1	L	$Q_{1s \rightarrow 2s}$		E_{max} (percent)	
		‡I	II	I	II
0.90	0	0.0529	0.523	0.40	0.40
1.00	0	0.0766	0.0768	0.12	0.60
0.90	1	0.0045	0.0048	2.3	10
1.00	1	0.0145	0.0147	0.33	1.3

*I and II refer to iterative and noniterative methods, respectively; E_{max} is the maximum of the error to value ratios in the reciprocity relation.
†See Reference 2.
‡See References 4 and 5.

iterative and noniterative methods, respectively; and E_{max} is the maximum of the error to value ratios in the reciprocity relations (Equation 83). In the 1s - 2s eigenstates coupling approximation the noniterative method is far more accurate than the iterative method and, as is seen, the cross sections by the two methods differ from each other sometimes in their first significant figure. In the 1s - 2s - 2p eigenstates coupling approximation, on the other hand, the results by the iterative method seems to be somewhat more accurate. The reason is contributed to the effect of the r^{-2} long-range potential, which appears in the differential equations when the 2p state is included in the eigenstates coupling approximation. Two different methods are used in References 4 and 5 and in the present paper to estimate the effect of this potential for large distances; and it may be that in References 4 and 5 this effect is better taken into account. Nevertheless the cross sections are the same in their first three decimal places.

In Figure 1 we present the theoretical and the experimental estimate of the $1s \rightarrow 2s$ excitation cross section. The calculated curves are Born, 1s - 2s coupling, 1s - 2s - 2p coupling exchange neglected, and 1s - 2s - 2p coupling exchange included approximation. The first three of these curves are the same as References 4 and 5. The experimental curves are those of Lichten and Schultz (Reference 18) and Stebbings, Fite, and Hummer (Reference 19). The various calculated results agree better with the results of Lichten and Schultz. However, recent calculations of Taylor and Burke (Reference 20) have shown that, in an eigenstates expansion calculation where 1s, 2s, 2p, 3s, and 3p are included, the cross section at the peak of the 1s - 2s - 2p curve is reduced by 30 percent. This suggests that, within the eigenstates expansion approximation, more states should be included to insure that the convergence has been achieved; and the discrepancy between the two experimental results is still an unresolved problem. As another theoretical approach to the problem, H. L. Kyle and A. Temkin (Reference 21) have extended the nonadiabatic theory of scattering developed by A. Temkin (Reference 22) to the $L = 0$, $1s \rightarrow 2s$ inelastic scattering of electrons by the hydrogen atom. They find a 30 percent decrease in the $1s \rightarrow 2s$ cross section as calculated by the 1s - 2s close coupling approximation.

Comparison of the exchange neglected and exchange included 1s - 2s - 2p coupling shows that exchange is mostly important at threshold, and its effect does not extend beyond 20 electron volts.

Table 2 gives the numerical values of the $1s \rightarrow 2s$ cross section in different approximations. The $1s \rightarrow 2s$ excitation cross section in the singlet state has an interesting behavior immediately above threshold. In Figure 2 this cross section for a range of 600 milli electron volts (mev) above threshold is plotted. In the $1s - 2s$ coupling approximation a maximum appears at 34 mev, while in the $1s - 2s - 2p$ coupling approximation there are three maxima of approximately the same magnitudes at 17, 34, and 87 mev, respectively. In the singlet case the cross section rises sharply within a range of 17 mev above threshold to a value of about $0.04 \pi a_0^2$; it then rises with an approximately constant and small slope. The contribution of the triplet case is seen to be almost negligible at the threshold, and it has no maximum in this region. It should be noted that the principal maximum in the $1s \rightarrow 2s$ excitation cross section appears at about 3 ev with a value of about 0.35, and has a contribution from a higher angular momentum than $L = 0$. Although no study has been made to relate the existence of the maxima above threshold to any physical phenomena, it may be said that, similar to resonances below threshold in the elastic scattering of electrons by the hydrogen atom, these maxima are due to formation of some unstable states of the negative hydrogen ion. The numerical values of the $1s \rightarrow 2s$ cross section at threshold are given in Table 3. Damburg and Peterkop (Reference 6), and Gailitis and Damburg (Reference 23) have made an extensive study of the behavior of different cross sections near threshold in the $1s - 2s$ and the $1s - 2s - 2p$ eigenstates coupling approximations.

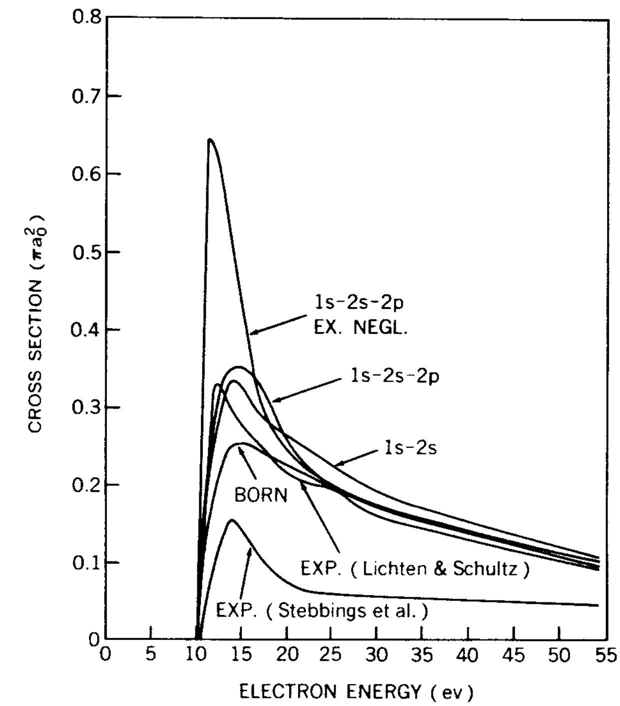

Figure 1 – $1s \rightarrow 2s$ total excitation cross section. ($1s - 2s$ refers to $1s - 2s$ eigenstates coupling approximation; $1s - 2s - 2p$ has similar meaning. EX. NEGL. refers to exchange neglected case, BORN is the Born approximation, and EXP. refers to experiment.)

In Figure 3 we have shown the $2s \rightarrow 2s$ elastic cross section. The $1s - 2s$ coupling approximation gives a value of $944 \pi a_0^2$ at zero incident energy, while the corresponding value in the Born approximation is $768 \pi a_0^2$. The high value of this cross section at zero energy is in sharp contrast with its geometrical cross section. The zero energy $2s \rightarrow 2s$ cross section in the $1s - 2s - 2p$ coupling approximation, because of the r^{-2} potential, is difficult to find. The $2s \rightarrow 2s$ cross section has certain maxima and minima at low energy which are not found in the $1s \rightarrow 1s$ cross section. Figure 4 shows the $L = 0$ singlet and triplet $2s \rightarrow 2s$ cross section in the two approximations. While there is one minimum in the $1s - 2s$ coupling approximation, there are three minima in the $1s - 2s - 2p$ coupling approximation. It is thought that the existence of these minima is due to a wider potential range in the $2s \rightarrow 2s$ scattering, a case which does not exist in the $1s \rightarrow 1s$

Table 2

1s → 2s Excitation Cross Section.

(a) Born approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.16376	0.00981	0.00021	0.00000	0.00000	0.00000	0.00000	0.00000	0.17378	0.17379
1.0	0.19578	0.04795	0.00428	0.00026	0.00000	0.00000	0.00000	0.00000	0.24827	0.24827
1.1	0.16272	0.07073	0.01141	0.00125	0.00011	0.00001	0.00000	0.00000	0.24622	0.24623
1.2	0.12704	0.07896	0.01858	0.00299	0.00039	0.00004	0.00000	0.00000	0.22800	0.22800
1.5	0.05872	0.06606	0.02979	0.00939	0.00242	0.00053	0.00010	0.00002	0.16703	0.16706
2.0	0.01946	0.03363	0.02521	0.01365	0.00614	0.00236	0.00081	0.00025	0.10151	0.10187
3.0	0.00388	0.00909	0.01019	0.00866	0.00628	0.00394	0.00226	0.00116	0.04546	0.04758
4.0	0.00123	0.00320	0.00420	0.00431	0.00385	0.00301	0.00216	0.00141	0.02337	0.02720

(b) Exchange neglected 1s - 2s - 2p eigenstates coupling approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.2202	0.0749	0.3535	--	--	--	--	--	0.6486	0.6486
1.0	0.1685	0.1427	0.1598	0.0517	--	--	--	--	0.5227	0.5227
1.1	0.0951	0.1142	0.0298	0.0616	0.0231	--	--	--	0.3238	0.3238
1.2	0.0594	0.1137	0.0032	0.0360	0.0244	0.0135	--	--	0.2502	0.2502
1.5	0.0249	0.0861	0.0201	0.0068	0.0112	0.0118	0.0074	--	0.1683	0.1683
2.0	0.0101	0.0373	0.0255	0.0107	0.0046	0.0034	0.0033	--	0.0949	0.0953

(c) 1s - 2s eigenstates coupling approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.9	0.0375	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	--	0.0392	---
1.0	0.0725	0.0583	0.0002	0.0000	0.0000	0.0000	0.0000	--	0.1310	
1.1	0.0701	0.0525	0.0023	0.0000	0.0000	0.0000	0.0000	--	0.1249	
1.2	0.0547	0.0534	0.0054	0.0002	0.0000	0.0000	0.0000	--	0.1137	
1.5	0.0241	0.0384	0.0110	0.0022	0.0004	0.0001	0.0000	--	0.0762	
2.0	0.0072	0.0157	0.0093	0.0041	0.0015	0.0005	0.0002	--	0.0385	

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0004	0.1686	0.0060	0.0000	0.0000	0.0000	0.0000	--	0.1750	0.2142	0.2142
1.0	0.0021	0.1528	0.0446	0.0021	0.0001	0.0000	0.0000	--	0.2017	0.3327	0.3327
1.1	0.0044	0.1052	0.0568	0.0068	0.0005	0.0000	0.0000	--	0.1737	0.2987	0.2987
1.2	0.0061	0.0737	0.0576	0.0114	0.0015	0.0002	0.0000	--	0.1505	0.2642	0.2642
1.5	0.0073	0.0355	0.0406	0.0174	0.0050	0.0012	0.0002	--	0.1072	0.1833	0.1833
2.0	0.0049	0.0162	0.0205	0.0143	0.0074	0.0032	0.0012	--	0.0677	0.1062	0.1068

(d) 1s - 2s - 2p eigenstates coupling approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.9	0.0523	0.0048	0.0620	--	--	--	--	--	0.1191	---
1.0	0.0768	0.0147	0.0833	0.0092	--	--	--	--	0.1840	
1.1	0.0585	0.0245	0.0647	0.0236	0.0055	--	--	--	0.1768	
1.2	0.0382	0.0251	0.0246	0.0252	0.0081	0.0028	--	--	0.1240	
1.5	0.0123	0.0308	0.0015	0.0041	0.0051	0.0034	0.0023	0.0026	0.0621	
2.0	0.0049	0.0152	0.0068	0.0021	0.0010	0.0010	0.0011	0.0008	0.0329	
3.0	0.0010	0.0031	0.0031	0.0023	0.0015	0.0009	0.0005	0.0006	0.0130	
4.0	0.0003	0.0010	0.0012	0.0012	0.0010	0.0008	--	--	0.0055	

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0013	0.0748	0.0019	--	--	--	--	--	0.0780	0.1971	0.1971
1.0	0.0040	0.1224	0.0195	0.0214	--	--	--	--	0.1673	0.3513	0.3513
1.1	0.0050	0.1013	0.0326	0.0077	0.0131	--	--	--	0.1597	0.3366	0.3366
1.2	0.0055	0.0724	0.0359	0.0036	0.0105	0.0076	--	--	0.1355	0.2596	0.2596
1.5	0.0045	0.0333	0.0309	0.0072	0.0046	0.0054	0.0049	0.0043	0.0951	0.1573	0.1573
2.0	0.0031	0.0155	0.0176	0.0101	0.0044	0.0025	0.0023	0.0019	0.0574	0.0903	0.0907
3.0	0.0013	0.0048	0.0065	0.0059	0.0044	0.0029	0.0018	0.0012	0.0288	0.0418	0.0439
4.0	0.0006	0.0019	0.0028	0.0030	0.0027	0.0022	--	--	0.0132	0.0187	0.0261

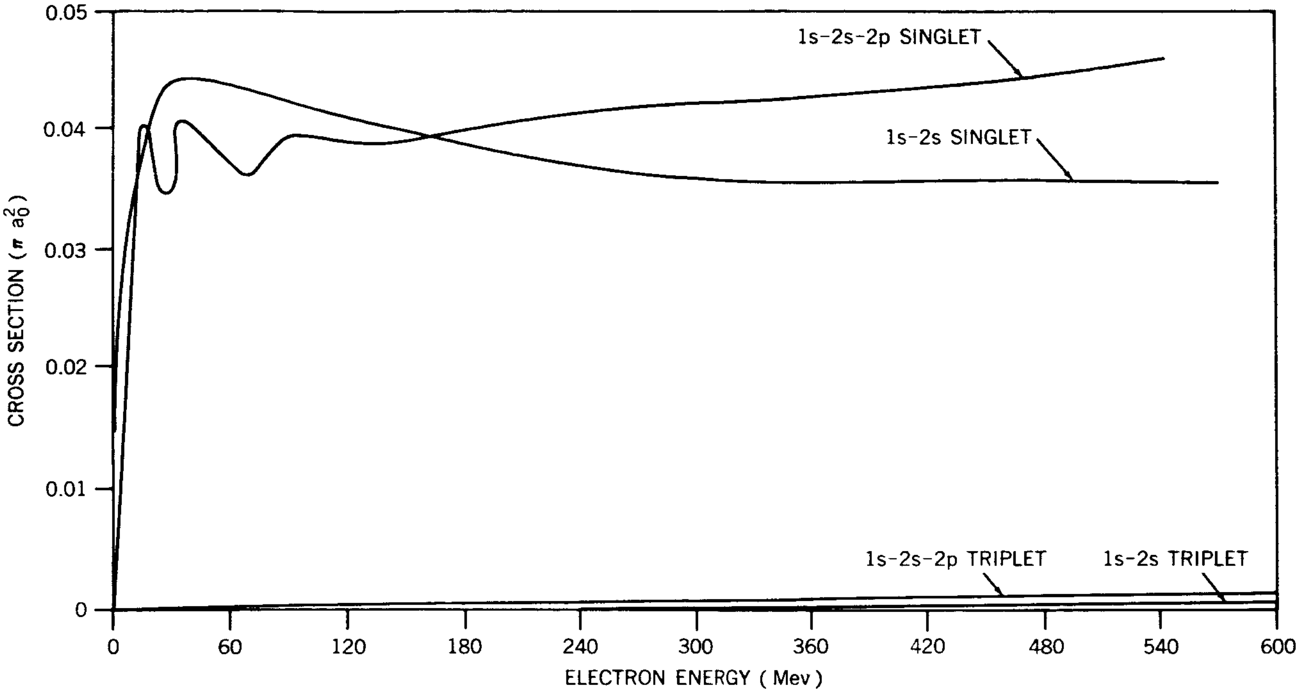

Figure 2 – L = 0, 1s → 2s excitation cross section above threshold. (The cross sections are given for the two spin states singlet and triplet, and for the two approximations 1s - 2s and 1s - 2s - 2p. The total cross section is the sum of the singlet and the triplet cross sections.)*

scattering. In Table 4 we have listed the numerical values of the 2s → 2s cross section in different approximations.

In Figure 5 the four calculated curves for the 1s → 2p excitation cross section are compared with the measurement of Fite, Stebbings, and Brackmann (References 24 and 25). The 1s - 2s - 2p and the Born curves are the same as in References 4 and 5, but the 1s - 2s - 2p exchange neglected and the 1s - 2p curves are not calculated in these references. As concluded before, the calculated curves are higher than the experimental. Moreover, we notice that, similar to the 1s → 2s excitation cross section, the inclusion of the exchange lowers the value of the cross section at threshold. Table 5 gives the numerical values of the 1s → 2p cross section in different approximations.

The calculation of the 2p → 2p elastic cross section is more complicated than the

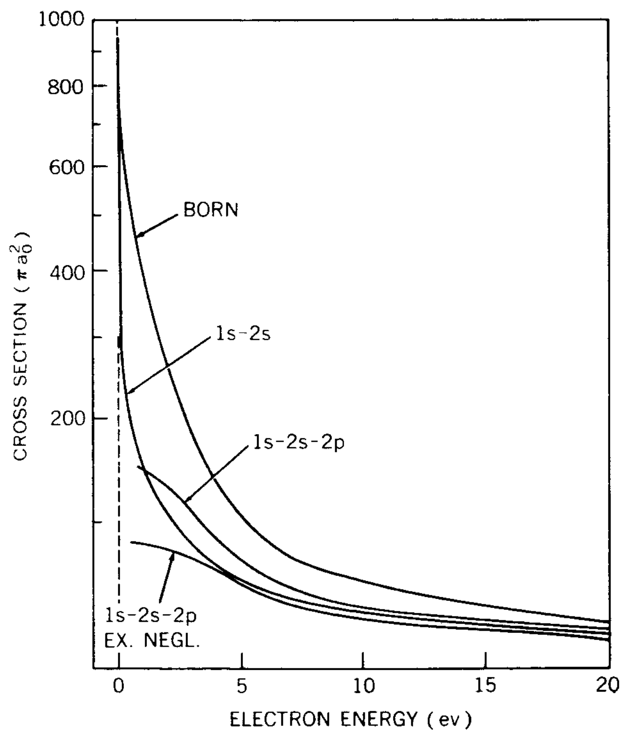

Figure 3 – 2s → 2s total elastic cross section. (Curves are designated as in Figure 1.)

*According to Gailitis and Damburg, when the energy difference between the 2s and 2p states is neglected in the 1s - 2s - 2p couplings, the 1s → 2s excitation cross section does not go to zero at threshold (see Reference 23, and Figure 2). Figures 2 and 4 show that in the 1s - 2s - 2p couplings, if E_{n-1} and E_n represent the energy with respect to the threshold of the two neighboring maxima or minima then $E_n/E_{n-1} \cong$ constant. This may be attributed to the r^{-2} potential, which is due to the coupling between the 2s and the 2p states. For further details, see Reference 23.

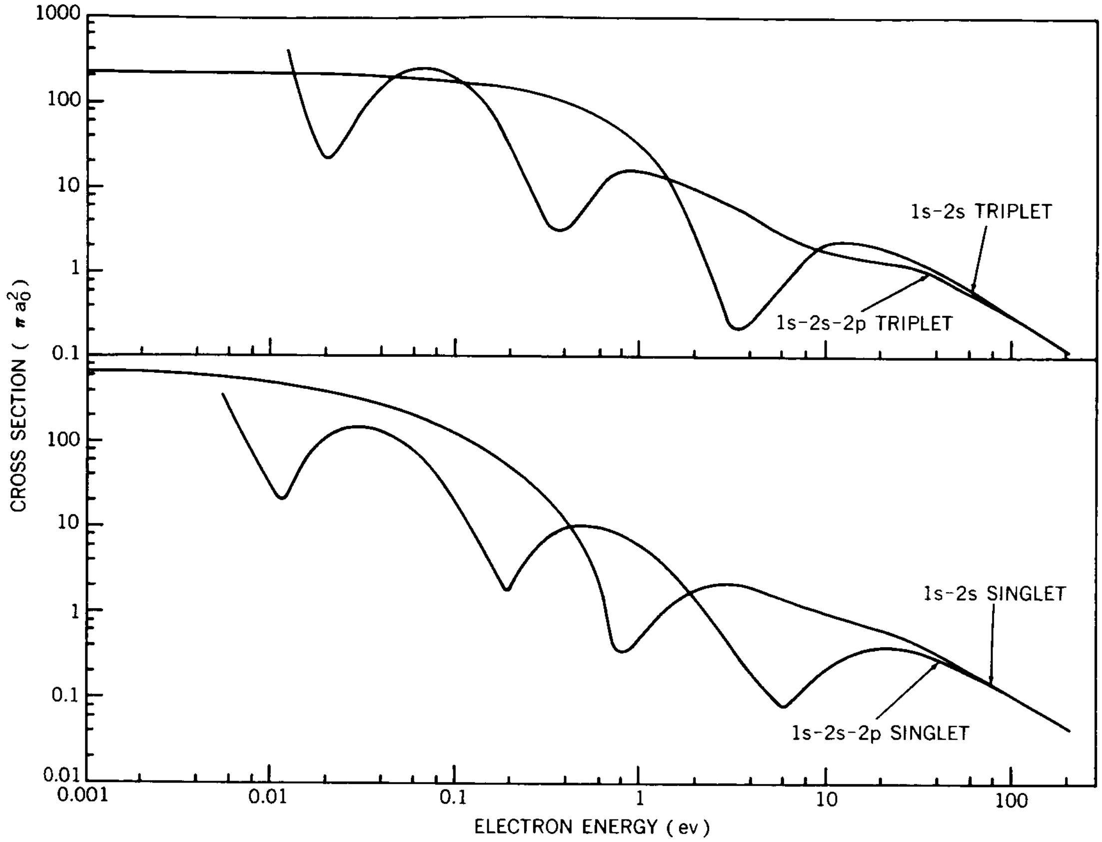

Figure 4 – L = 0, 2s → 2s elastic cross section. (Curves are designated as in Figure 2.)

Table 3

The Singlet L = 0, 1s → 2s Excitation Cross Section Near Threshold.*

k_2	0	0.01	0.02	0.025	0.030	0.035	0.04
E(mev)	0	1.36	5.44	8.50	12.2	16.7	21.8
Q_1	0	0.0168	0.0298	--	0.0377	--	0.0423
Q_2	0	--	0.0149	0.0259	0.0349	0.0405	0.0353
k_2	0.045	0.050	0.060	0.070	0.080	0.090	0.100
E(mev)	27.5	34.0	49.0	66.6	87.0	110.	136.
Q_1	--	0.0446	0.0441	0.0435	0.0423	0.0412	0.0405
Q_2	0.0346	0.0405	0.0391	0.0361	0.0395	0.0392	0.0385

*k_2 is the wave number of the inelastically scattered wave, and E is the corresponding energy in mev; Q_1 and Q_2 are the cross sections according to the 1s - 2s and the 1s - 2s - 2p couplings, respectively.

Table 4
2s - 2s Elastic Cross Section.

(a) Born approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.24	389.97	15.910	0.27680	0.00319	0.00003	0.00000	0.00000	0.00000	406.16	406.17
0.50	105.52	32.129	5.0152	0.55306	0.04846	0.00347	0.00022	0.00001	143.269	143.276
0.68	47.381	24.746	7.4981	1.7023	0.31602	0.04869	0.00658	0.00078	81.700	81.703
0.83	26.562	17.895	7.5601	2.5080	0.69820	0.16365	0.03393	0.00621	55.427	55.440
1.23	8.2461	7.6846	4.9702	2.7483	1.3500	0.57745	0.22452	0.07803	25.879	25.990
1.80	2.4331	2.7773	2.2763	1.6805	1.1541	0.71994	0.41776	0.22120	11.680	12.105
2.87	0.5245	0.71381	0.68903	0.61123	0.51876	0.41048	0.31076	0.21860	4.0011	4.8280
3.91	0.18794	0.27611	0.28658	0.27339	0.25098	0.21580	0.17946	0.14029	1.8106	2.7417

(b) Exchange neglected 1s - 2s - 2p eigenstates coupling approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.24	32.02	8.489	42.26	--	--	--	--	--	82.77	82.78
0.50	2.041	7.710	23.35	9.004	9.368	7.702	5.870	--	65.045	65.052
0.68	2.255	8.247	15.16	5.547	4.373	3.755	2.975	--	42.312	42.316
0.83	1.861	8.206	10.67	4.637	2.792	2.223	1.818	--	32.207	32.226
1.23	1.716	4.987	5.030	3.321	1.797	1.058	0.7179	--	18.537	18.726
1.80	1.020	2.134	2.150	1.750	1.275	0.8320	0.5457	--	9.707	10.352

(c) 1s - 2s eigenstates coupling approximation

Singlet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.24	0.3303	8.196	0.2628	0.0028	--	--	--	--	8.792	---
0.50	1.532	10.38	0.0275	0.0048	0.0008	0.0002	0.0249	--	11.97	
0.68	1.115	5.536	1.502	0.1150	0.0087	0.0010	0.0017	--	8.279	
0.83	0.8980	3.512	1.997	0.4303	0.0747	0.0129	0.0032	--	6.928	
1.23	0.5702	1.413	1.236	0.7010	0.3129	0.1228	0.0450	--	4.401	
1.80	0.2825	0.5370	0.5285	0.4193	0.2931	0.1863	0.1110	--	2.358	

Triplet										$\Sigma_S + \Sigma_T$	Q_T
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T		
0.24	45.94	118.8	7.713	0.0540	--	--	--	--	172.51	181.30	181.31
0.50	0.2102	34.44	21.05	2.776	0.2521	0.0316	0.0994	--	58.86	70.83	70.84
0.68	1.366	18.13	12.74	4.059	0.8282	0.1463	0.0442	--	37.31	45.60	45.60
0.83	2.112	11.65	8.725	3.887	1.230	0.3225	0.0850	--	28.01	34.94	34.96
1.23	1.811	4.691	4.008	2.585	1.399	0.6637	0.2862	--	15.44	19.84	20.03
1.80	0.8989	1.735	1.652	1.316	0.9510	0.6359	0.4008	--	7.590	9.947	10.592

(d) 1s - 2s - 2p eigenstates coupling approximation

Singlet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.24	7.800	14.79	22.42	--	--	--	--	--	45.01	---
0.50	0.2858	0.6960	3.149	4.447	2.925	2.063	1.491	--	15.057	
0.68	0.0661	1.044	2.455	1.884	1.480	1.098	0.7928	--	8.820	
0.83	0.1675	1.088	2.105	0.9905	0.8282	0.6606	0.5071	--	6.347	
1.23	0.3739	1.075	1.196	0.7196	0.3940	0.2496	0.1827	0.1409	4.332	
1.80	0.2416	0.4974	0.5133	0.4133	0.2923	0.1928	0.1247	0.0799	2.3553	
2.87	0.0847	0.1489	0.1574	0.1466	0.1280	0.1057	0.0852	0.0658	0.9223	
3.91	0.0365	0.0635	0.0702	0.0698	0.0660	0.0599	--	--	0.3659	

Triplet										$\Sigma_S + \Sigma_T$	Q_T
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T		
0.24	16.52	1.236	89.65	--	--	--	--	--	107.41	152.42	152.43
0.50	6.172	17.19	30.69	12.90	5.559	5.373	4.257	--	82.14	97.206	97.213
0.68	2.346	12.88	14.52	7.937	3.046	2.459	2.090	--	45.28	54.099	54.103
0.83	1.709	9.166	8.976	5.367	2.365	1.514	1.246	--	30.343	36.686	36.705
1.23	1.391	4.199	3.880	2.681	1.585	0.9110	0.5658	0.4094	15.622	19.955	20.066
1.80	0.7898	1.656	1.603	1.291	0.9466	0.6520	0.4305	0.2786	7.648	10.002	10.427
2.87	0.2622	0.4652	0.4857	0.4479	0.3901	0.3234	0.2623	0.2045	2.8413	3.7636	4.5905
3.91	0.1113	0.1945	0.2146	0.2122	0.2000	0.1812	--	--	1.1138	1.4797	2.7306

Table 5
1s → 2p Excitation Cross Section.

(a) Born approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.00107	0.46700	0.09607	0.01025	0.00087	0.00007	0.00001	0.00000	0.56534	0.57535
1.0	0.00499	0.48867	0.35645	0.13467	0.03964	0.01032	0.00254	0.00059	1.03787	1.03851
1.1	0.00702	0.36207	0.41698	0.24992	0.11533	0.04649	0.01753	0.00624	1.22158	1.22859
1.2	0.00747	0.25540	0.38137	0.29903	0.17908	0.09269	0.04453	0.02004	1.27961	1.30741
1.5	0.00550	0.09184	0.19986	0.23775	0.21386	0.16292	0.11291	0.07232	1.09696	1.28101
2.0	0.00234	0.02222	0.05938	0.09386	0.11287	0.11376	0.10248	0.08374	0.59065	1.04055
3.0	0.00048	0.00285	0.00806	0.01537	0.02309	0.02920	0.03271	0.03273	0.14449	0.66256
4.0	0.00013	0.00066	0.00179	0.00359	0.00586	0.00816	0.01009	0.01114	0.04142	0.45252

(b) Exchange neglected 1s - 2s - 2p eigenstates coupling approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.1600	0.3985	0.6497	--	--	--	--	--	1.2082	1.2194
1.0	0.1007	0.2917	0.8190	0.2190	0.0476	0.0224	--	--	1.5004	1.5041
1.1	0.0980	0.2008	0.6201	0.3696	0.1380	0.0586	0.0166	--	1.5017	1.5150
1.2	0.0822	0.1251	0.4481	0.3922	0.2044	0.1014	0.0403	--	1.3937	1.4416
1.5	0.0372	0.0334	0.1671	0.2568	0.2295	0.1706	0.1136	--	1.0082	1.2645
2.0	0.0105	0.0068	0.0394	0.0837	0.1089	0.1165	0.1042	--	0.4700	1.0036

(c) 1s - 2p eigenstates coupling approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.9	0.0044	0.1216	0.1422	--	--	--	--	--	0.2682	---
1.0	0.0168	0.0655	0.3011	0.0206	0.0057	0.0059	--	--	0.4156	
1.1	0.0299	0.0366	0.3948	0.0851	0.0260	0.0099	0.0060	--	0.5883	
1.2	0.0296	0.0169	0.3088	0.1421	0.0517	0.0236	0.0103	--	0.5830	
1.5	0.0059	0.0037	0.0821	0.0989	0.0718	0.0458	0.0304	--	0.3386	
2.0	0.0010	0.0006	0.0131	0.0271	0.0327	0.0335	0.0296	--	0.1376	

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0002	0.2066	0.0005	--	--	--	--	--	0.2073	0.4755	0.4867
1.0	0.0016	0.1078	0.0020	0.1651	0.0363	0.0187	--	--	0.3315	0.7471	0.7508
1.1	0.0037	0.0540	0.0060	0.1599	0.1002	0.0365	0.0217	--	0.3820	0.9703	0.9836
1.2	0.0055	0.0249	0.0098	0.1446	0.1336	0.0695	0.0341	--	0.4220	1.0050	1.0529
1.5	0.0059	0.0027	0.0133	0.0868	0.1231	0.1100	0.0849	--	0.4267	0.7652	1.0215
2.0	0.0028	0.0002	0.0073	0.0311	0.0559	0.0700	0.0772	--	0.2445	0.3820	0.9156

(d) 1s - 2s - 2p eigenstates coupling approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S	---
0.9	0.0390	0.0745	0.1027	--	--	--	--	--	0.2162	---
1.0	0.0360	0.1123	0.2575	0.0317	--	--	--	--	0.4375	
1.1	0.0358	0.1094	0.3405	0.0886	0.0308	0.0113	0.0075	--	0.6239	
1.2	0.0345	0.0806	0.2912	0.1278	0.0506	0.0237	0.0105	--	0.6189	
1.5	0.0172	0.0175	0.0953	0.1003	0.0693	0.0440	0.0290	0.0238	0.3964	
2.0	0.0036	0.0023	0.0170	0.0303	0.0344	0.0333	0.0293	0.0229	0.1731	
3.0	0.0004	0.0002	0.0015	0.0037	0.0060	0.0078	0.0094	0.0106	0.0396	
4.0	0.0001	0.0001	0.0003	0.0008	0.0014	0.0020	--	--	0.0047	

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0007	0.0682	0.0112	--	--	--	--	--	0.0801	0.2963	0.3075
1.0	0.0033	0.0801	0.0500	0.1730	--	--	--	--	0.3064	0.7439	0.7976
1.1	0.0070	0.0626	0.0567	0.1841	0.1082	0.0404	0.0209	--	0.4799	1.1039	1.1172
1.2	0.0096	0.0418	0.0537	0.1761	0.1409	0.0729	0.0332	--	0.5282	1.1471	1.1950
1.5	0.0107	0.0131	0.0351	0.1081	0.1343	0.1157	0.0842	0.0596	0.5608	0.9570	1.1410
2.0	0.0053	0.0038	0.0143	0.0393	0.0625	0.0731	0.0738	0.0642	0.3363	0.5094	0.9593
3.0	0.0010	0.0006	0.0025	0.0066	0.0122	0.0175	0.0220	0.0246	0.0870	0.1266	0.6095
4.0	0.0002	0.0002	0.0006	0.0016	0.0031	0.0048	--	--	0.0105	0.0152	0.4475

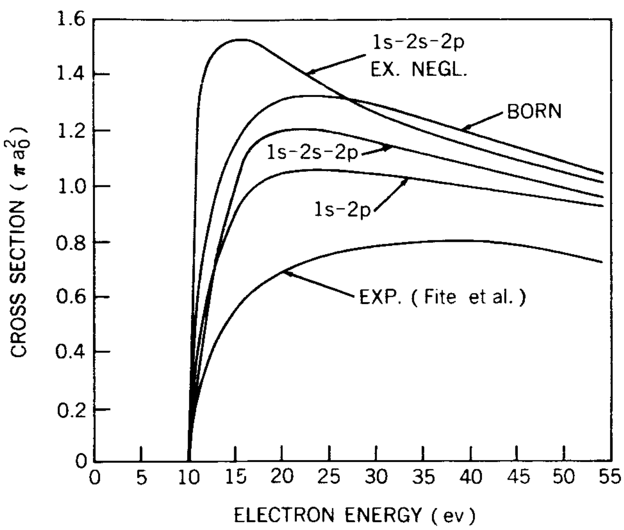

Figure 5 — 1s → 2p total excitation cross section. (1s - 2p refers to 1s - 2p eigenstates coupling approximation; 1s - 2s - 2p has similar meaning. EX. NEGL. refers to exchange neglected case, BORN is the Born approximation, and EXP. refers to experiment.)

cases so far considered. For a given total angular momentum L, the angular momentum of the partial wave which is scattered from the 2p state may be L - 1, L, and L + 1. The first and the third values correspond to a wave function which has the same parity as the wave functions in the 1s and the 2s channels; in this case, $L - \ell_1 - \ell_2$ is even. The second value corresponds to a wave function with a different parity, and the only process that occurs with this parity is the 2p elastic scattering; in this case, $L - \ell_1 - \ell_2$ is odd. We have calculated the 2p → 2p cross sections for the two cases, and they are listed in Table 6. The total cross section is shown in Figure 6 (on page 33). Because of the r^{-2} potential it is difficult to find the zero energy value of this cross section.

The 2s → 2p transition cross section has application in some plasma and stellar atmosphere calculations. The total cross section using the Born approximation is given by Seaton (Reference 26). In Table 7 (on page 32) we list the partial cross section using the close coupling approximation. This table may be found useful in problems in which plasma shielding occurs, where only electrons with an impact parameter with a given range can induce the 2s → 2p transition.

It may be noted that the cross sections for the inverse processes 2s → 1s, 2p → 1s, and 2p → 2s may be calculated by Equation 35 and the symmetry of the T-matrix.

In all the tables listed here, k_1 is the wave number in the 1s, and k_2 is the wave number in the 2s or the 2p channels. The energy, in electron volts, of the incident electron in each channel is given by $E = 13.6\, k^2$, where k could be k_1 or k_2. All cross sections are in units of πa_0^2. In the different tables, Σ is the sum of the partial cross sections calculated. The total cross section Q_T is obtained by adding the contribution of higher partial waves than those calculated using the regular Born approximation; this could easily be done with the help of the table of the Born approximation.

CONCLUSION

The noniterative technique employed here can be applied to a large class of problems containing exchange integrals. The method is particularly useful when the exchange potential is comparable to the direct potential, in which case the convergence of iteration is slow.

Table 6

2p → 2p Elastic Cross Section.

(a) L − ℓ_1 − ℓ_2 odd, Born approximation

k_2	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_0
0.24	26.562	6.1961	2.1260	0.92680	0.44497	0.22694	0.08105	36.56
0.50	14.210	5.2190	2.1768	1.0526	0.55433	0.31476	0.18383	23.71
0.68	8.8346	4.0761	1.9476	1.0100	0.54983	0.31728	0.18718	16.923
0.83	6.0065	3.2062	1.6993	0.94122	0.53204	0.31331	0.18680	12.8854
1.23	2.5053	1.7048	1.1013	0.70920	0.44518	0.28212	0.17577	6.9237
1.80	0.91169	0.74615	0.56949	0.42475	0.30158	0.21122	0.14245	3.30733
2.87	0.23647	0.22647	0.20035	0.17178	0.13878	0.10926	0.08177	1.16488

(b) L − ℓ_1 − ℓ_2 odd, exchange neglected 2p eigenstates coupling approximations

k_2	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_0
0.24	61.12	8.444	2.5808	1.1408	0.6200	0.3720	0.2516	74.52
0.50	15.292	6.884	2.5436	1.1580	0.6216	0.3640	0.2352	27.10
0.68	8.008	4.940	2.2548	1.1160	0.6160	0.3640	0.2352	17.54
0.83	5.108	3.6364	1.9292	1.0380	0.5968	0.3592	0.2340	12.90
1.23	2.0484	1.7392	1.1812	0.7652	0.4972	0.3236	0.2208	6.776
1.80	0.7640	0.7220	0.5816	0.4436	0.3312	0.2400	0.1784	3.261
2.87	0.2132	0.2180	0.2004	0.1776	0.1520	0.1272	0.1064	1.195

(c) L − ℓ_1 − ℓ_2 odd, 2p eigenstates coupling approximation

Singlet								
k_2	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{0S}
0.24	2.963	4.161	0.6725	0.2861	0.1552	0.0930	0.0629	8.394
0.50	3.735	3.182	0.7915	0.3066	0.1576	0.0913	0.0589	8.323
0.68	2.165	1.728	0.6851	0.3025	0.1587	0.0920	0.0590	5.190
0.83	1.371	1.107	0.5562	0.2799	0.1547	0.0913	0.0589	3.619
1.23	0.5280	0.4603	0.3115	0.1991	0.1277	0.0823	0.0558	1.7647
1.80	0.1928	0.1831	0.1475	0.1124	0.0837	0.0605	0.0449	0.8249
2.87	0.0534	0.0547	0.0503	0.0445	0.0381	0.0319	0.0267	0.2996
Triplet								
k_2	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{0T}
0.24	49.22	3.265	1.850	0.8528	0.4650	0.2788	0.1886	56.12
0.50	7.791	1.851	1.504	0.8193	0.4598	0.2722	0.1764	12.87
0.68	4.720	2.219	1.361	0.7700	0.4481	0.2700	0.1756	9.964
0.83	3.373	2.099	1.237	0.7198	0.4318	0.2652	0.1744	8.300
1.23	1.484	1.225	0.8376	0.5509	0.3630	0.2384	0.1639	4.863
1.80	0.5674	0.5337	0.4295	0.3283	0.2456	0.1784	0.1330	2.4159
2.87	0.1596	0.1632	0.1500	0.1328	0.1136	0.0951	0.0797	0.8940

(d) L − ℓ_1 − ℓ_2 even, Born approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_E	Q_T
0.24	12.488	230.42	4.0427	1.9014	0.30797	0.57480	0.29675	0.06128	250.09	290.69
0.50	0.1758	74.475	7.0963	0.92172	0.48094	0.45745	0.30098	0.05695	83.965	109.714
0.68	0.07386	36.478	6.5573	1.0156	0.29902	0.27895	0.23113	0.04364	44.978	63.742
0.83	0.22032	21.559	5.4143	1.1653	0.26124	0.15835	0.15225	0.02533	28.956	43.572
1.23	0.25024	7.3349	2.9703	1.1453	0.37750	0.11091	0.04377	0.03572	12.269	20.571
1.80	0.13477	2.3518	1.3155	0.74676	0.39290	0.18754	0.07731	0.02824	5.2348	9.6066
2.87	0.04395	0.55809	0.40443	0.30267	0.21866	0.15188	0.09753	0.05832	1.8355	3.8272
3.91	0.01868	0.20876	0.17048	0.14307	0.11656	0.09255	0.06896	0.04864	0.8677	2.1455

(e) L − ℓ_1 − ℓ_2 even, exchange neglected 1s − 2s − 2p eigenstates coupling approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_E	Q_T
0.24	31.96	91.21	154.6	92.86	55.86	36.79	24.37	--	487.7	566.32
0.50	9.371	12.65	30.88	20.53	12.99	8.451	5.695	--	100.6	129.8
0.68	4.156	5.953	13.19	9.628	6.563	4.508	3.130	--	47.13	66.56
0.83	2.542	4.560	7.424	5.249	3.811	2.793	2.032	--	28.41	43.07
1.23	1.208	2.879	2.906	1.734	1.106	0.8438	0.6912	--	11.37	19.56
1.80	0.5612	1.385	1.238	0.8299	0.5109	0.3005	0.2022	--	5.028	9.382

Table 6 (Concluded)
2p - 2p Elastic Cross Section.

(f) $L - \ell_1 - \ell_2$ even, 1s - 2p eigenstates coupling approximation

Singlet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ES}	---
0.24	1.964	5.238	17.34	1.260	0.4896	0.2460	--	--	26.54	---
0.50	0.5131	3.159	1.544	1.439	0.4063	0.1906	0.1133	--	7.365	
0.68	0.2346	2.091	1.039	0.4944	0.2539	0.1520	0.0984	--	4.363	
0.83	0.1227	1.252	0.9930	0.1532	0.1191	0.0990	0.0766	--	2.816	
1.23	0.1071	0.6796	0.6167	0.2249	0.0635	0.0249	0.0217	--	1.7384	
1.80	0.0571	0.3366	0.2926	0.1818	0.0954	0.0426	0.0172	--	1.0233	
Triplet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ET}	Q_T
0.24	15.62	26.72	32.44	6.674	1.252	0.7359	--	--	83.44	178.89
0.50	4.844	3.384	19.97	12.52	0.8285	0.3266	0.2754	--	42.15	72.80
0.68	2.247	3.886	10.33	5.922	1.035	0.2270	0.1764	--	23.82	45.22
0.83	1.293	3.650	6.287	3.476	0.9248	0.2097	0.1162	--	15.957	32.45
1.23	0.4842	2.287	2.424	1.418	0.6072	0.2079	0.0717	--	7.500	17.28
1.80	0.1909	1.063	0.9673	0.6659	0.4001	0.2024	0.0962	--	3.586	8.943

(g) $L - \ell_1 - \ell_2$ even, 1s - 2s - 2p eigenstates coupling approximation

Singlet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ES}	---
0.24	7.852	13.45	38.56	21.41	15.44	8.610	6.432	--	111.75	---
0.50	2.470	5.026	7.433	4.900	3.201	2.101	1.417	--	26.548	
0.68	1.344	2.283	3.025	2.683	1.756	1.166	0.7903	--	13.047	
0.83	0.7424	1.316	1.579	1.518	1.079	0.7580	0.5313	--	7.524	
1.23	0.2813	0.6752	0.6254	0.3663	0.2726	0.2289	0.1916	--	2.641	
1.80	0.1357	0.3339	0.2862	0.1816	0.1065	0.0659	0.0471	0.0383	1.1952	
2.87	0.0513	0.1053	0.0930	0.0739	0.0553	0.0391	0.0268	0.0181	0.4628	
3.91	0.0267	0.0451	0.0422	0.0373	0.0318	0.0261	0.0212	0.0166	0.2470	
Triplet										
k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ET}	Q_T
0.24	27.90	75.79	63.10	87.21	41.31	26.12	17.13	--	338.56	518.92
0.50	4.337	4.540	20.66	21.62	10.38	6.373	4.255	--	72.17	122.01
0.68	2.823	4.018	10.75	8.986	5.149	3.337	2.302	--	37.37	67.46
0.83	2.032	3.674	6.400	4.796	2.950	2.013	1.468	--	23.333	44.54
1.23	0.9741	2.290	2.465	1.599	0.9568	0.6421	0.4924	--	9.419	20.11
1.80	0.4291	1.055	0.9303	0.6614	0.4150	0.2540	0.1639	0.1180	4.027	9.531
2.87	0.1564	0.3217	0.2907	0.2330	0.1780	0.1291	0.0907	0.0623	1.4619	3.945
3.91	0.0805	0.1366	0.1285	0.1143	0.0982	0.0810	0.0655	0.0524	0.7570	--

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I am indebted to Dr. A. Temkin for many fruitful and illuminating discussions. I also wish to thank Prof. Myers of the University of Maryland for a clarifying discussion.

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Table 7
2s → 2p Excitation Cross Section.

(a) Born approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	Σ	*Q_T
0.245	210.45	465.14	449.77	343.68	148.60	209.74	158.31	1985.69	13560
0.500	6.2469	30.729	57.561	64.948	54.469	49.590	40.391	303.935	3465.0
0.678	0.92003	6.6619	16.736	24.356	25.702	24.598	21.122	120.096	1930.9
0.831	0.24580	2.1480	6.4066	11.011	13.641	14.135	12.973	60.560	1308.4
1.225	0.02039	0.20887	0.78437	1.7481	2.7859	3.6015	3.9501	13.099	620.51
1.803	0.00187	0.01900	0.07823	0.20201	0.38645	0.59807	0.78354	2.0692	294.95
2.872	0.00011	0.00107	0.00444	0.01211	0.02545	0.04450	0.06688	0.15456	120.26
3.905	0.00002	0.00017	0.00067	0.00182	0.00389	0.00699	0.01096	0.02452	66.509

(b) Exchange neglected 1s - 2s - 2p eigenstates coupling approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	Σ	Q_T
0.245	5.311	12.59	23.21	--	--	--	--	41.11	12476
0.500	0.8651	10.55	1.143	18.92	26.25	--	--	57.73	3308.8
0.678	1.150	5.907	0.5760	7.168	12.28	14.46	15.08	56.62	1867.4
0.831	1.249	2.859	0.3831	3.158	6.664	8.591	9.391	32.295	1280.1
0.225	0.3847	0.4266	0.0881	0.4560	1.403	2.328	3.022	8.108	615.52
1.803	0.0654	0.0516	0.0142	0.0553	0.1846	0.3930	0.6183	1.3824	294.26

(c) 1s - 2s - 2p eigenstates coupling approximation

Singlet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	Σ_S	---
0.245	2.243	4.424	3.276	--	--	--	--	9.943	---
0.500	0.1241	1.605	1.348	6.360	7.159	--	--	16.596	
0.678	0.0362	1.446	0.5518	3.056	3.693	3.911	--	12.694	
0.831	0.1866	0.9881	0.2615	1.488	2.144	2.433	2.505	10.006	
1.225	0.1048	0.1516	0.0384	0.1639	0.4584	0.7031	0.8529	2.473	
1.803	0.0175	0.0157	0.0046	0.0148	0.0530	0.1108	0.1726	0.3890	
2.872	0.0014	0.0010	0.0004	0.0010	0.0032	0.0075	0.0133	0.0278	
3.905	0.0002	0.0002	0.0001	0.0002	0.0005	0.0012	0.0019	0.0043	

Triplet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.245	0.0000	10.40	56.74	--	--	--	--	67.14	77.083	12512
0.500	2.322	7.125	2.357	3.838	17.01	--	--	32.652	49.248	3300.3
0.678	1.590	2.363	0.3333	1.442	6.810	9.868	--	22.406	35.100	1867.0
0.831	0.9885	1.125	0.1226	0.8444	3.411	5.518	6.556	18.566	28.572	1276.4
1.225	0.2648	0.2173	0.0402	0.2297	0.7623	1.423	1.987	4.924	7.397	614.8
1.803	0.0455	0.0310	0.0094	0.0383	0.1223	0.2544	0.4070	0.9079	1.297	294.18
2.872	0.0040	0.0024	0.0009	0.0031	0.0095	0.0208	0.0359	0.0766	0.1044	120.21
3.905	0.0007	0.0004	0.0002	0.0005	0.0015	0.0035	0.0063	0.0131	0.0174	66.502

$$^{*}Q_T = \frac{72}{k_2^2}\left[14.8451 - \mu + \ln k_2^2\right], \quad \mu = \frac{2}{7}\left(1 - \frac{1}{\eta^7}\right) + \frac{1}{2}\sum_{n=1}^{5}\frac{1-\eta^{-n}}{n} + \frac{1}{2}\ln\eta, \quad \eta = 1 + 4k_2^2$$ (Reference 26).

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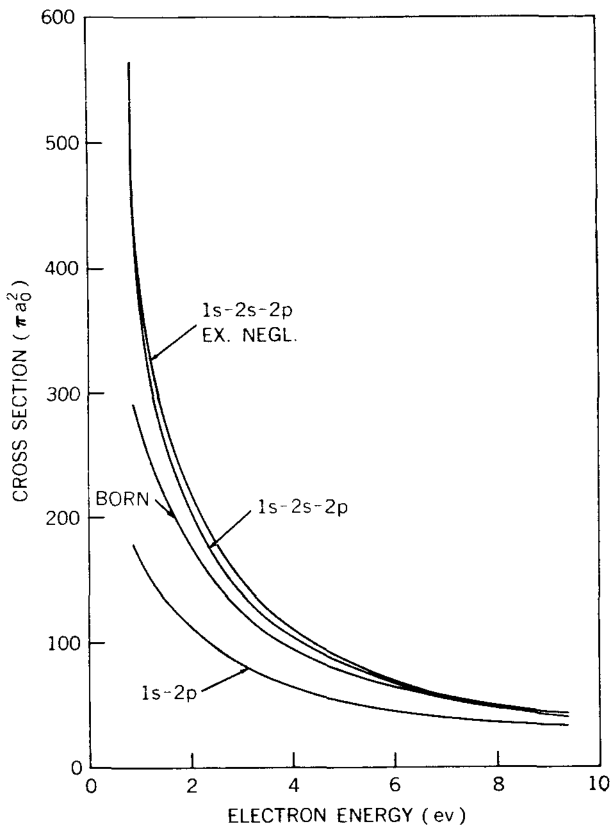

Figure 6 – 2p 2p total elastic cross sections. (Curves are designated as in Figure 5. The cross section at zero energy is finite but is not found here.)

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Appendix A

The Four Differential Equations

$$\left[\frac{d^2}{dr^2} + k_1^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u(k_1 L, r)$$

$$\begin{aligned}
= \; & 2y_0 (1s\,1s, r)\, u(k_1 L, r) + 2y_0 (1s\,2s, r)\, u(k_2 L, r) \\
& + 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1 (1s\,2p, r)\; u(k_2 L-1, r) \\
& - 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1 (1s\,2p, r)\; u(k_2 L+1, r) \\
& + \frac{2\beta}{2L+1}\, rR_{10}(r)\, y_L (1s\,k_1 L, r) + \frac{2\beta}{2L+1}\, rR_{20}(r)\, y_L (1s\,k_2 L, r) \\
& + 2\beta\left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{21}(r)\, y_{L-1} (1s\,k_2 L-1, r) \\
& - 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{21}(r)\, y_{L+1} (1s\,k_2 L+1, r) \\
& - \beta\delta(L, 0)\left(1 + k_1^2\right)\left(1s|k_1 L\right) rR_{10}(r) \\
& - \beta\delta(L, 0)\left(1 + k_2^2\right)\left(1s|k_2 L\right) rR_{20}(r) \\
& - \beta\delta(L-1, 0)\left(1 + k_2^2\right)\left(1s|k_2 L-1\right) rR_{21}(r)
\end{aligned} \tag{A1}$$

$$\left[\frac{d^2}{dr^2} + k_2^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u\left(k_2 L, r\right)$$

$$= 2y_0 \;(1s\,2s,\, r)\, u\left(k_1 L, r\right) + 2y_0 \;(2s\,2s,\, r)\, u\left(k_2 L, r\right)$$

$$+ 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1\,(2s\,2p,\, r)\; u\left(k_2 L-1,\, r\right)$$

$$- 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1\,(2s\,2p,\, r)\; u\left(k_2 L+1,\, r\right)$$

$$+ \frac{2\beta}{2L+1}\, rR_{10}(r)\, y_L\left(2s\, k_1 L,\, r\right) + \frac{2\beta}{2L+1}\, rR_{20}(r)\, y_L\left(2s\, k_2 L,\, r\right)$$

$$+ 2\beta\left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{21}(r)\, y_{L-1}\left(2s\, k_2 L-1,\, r\right)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{21}(r)\, y_{L+1}\left(2s\, k_2 L+1,\, r\right)$$

$$- \beta\delta(L,\, 0)\left(\frac{1}{4} + k_1^2\right)\left(2s|k_1 L\right) rR_{10}(r)$$

$$- \beta\delta(L,\, 0)\left(\frac{1}{4} + k_2^2\right)\left(2s|k_2 L\right) rR_{20}(r)$$

$$- \beta\delta(L-1,\, 0)\left(\frac{1}{4} + k_2^2\right)\left(2s|k_2 L-1\right) rR_{21}(r)\;. \qquad \text{(A2)}$$

$$\left[\frac{d^2}{dr^2} + k_2^2 - \frac{(L-1)L}{r^2} + \frac{2}{r}\right] u\left(k_2\, L-1,\ r\right)$$

$$= 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1\,(1s\ 2p,\ r)\, u\left(k_1\, L,\ r\right) + 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1\,(2s\ 2p,\ r)\ u\left(k_2\, L,\ r\right)$$

$$+\ 2\left[y_0\,(2p\ 2p,\ r) + \frac{L-1}{5(2L+1)}\, y_2\,(2p\ 2p,\ r)\right] u\left(k_2\, L-1,\ r\right)$$

$$-\ \frac{6}{5}\frac{\sqrt{L(L+1)}}{2L+1}\, y_2\,(2p\ 2p,\ r)\, u\left(k_2\, L+1,\ r\right)$$

$$+\ 2\beta\left[\frac{3L}{(2L+1)\,(2L-1)^2}\right]^{1/2} rR_{10}\,(r)\, y_{L-1}\,\left(2p\, k_1\, L,\ r\right)$$

$$+\ 2\beta\left[\frac{3L}{(2L+1)\,(2L-1)^2}\right]^{1/2} rR_{20}\,(r)\, y_{L-1}\,\left(2p\, k_2\, L,\ r\right)$$

$$+\ \frac{6\beta}{2L-1}\, rR_{21}\,(r)\left[\frac{y_L\,\left(2p\, k_2\, L-1,\ r\right)}{(2L+1)^2} + \frac{L-1}{2L-3}\, y_{L-2}\,\left(2p\, k_2\, L-1,\ r\right)\right]$$

$$-\ \frac{6\beta\sqrt{L(L+1)}}{(2L+1)^2}\, y_L\,\left(2p\, k_2\, L+1,\ r\right)\, rR_{21}\,(r)$$

$$-\ \beta\delta(L,\ 1)\left(\frac{1}{4} + k_1^2\right)\left(2p|k_1\, L\right) rR_{10}\,(r)$$

$$-\ \beta\delta(L,\ 1)\left(\frac{1}{4} + k_2^2\right)\left(2p|k_2\, L\right) rR_{20}\,(r)$$

$$-\ \beta\delta(L,\ 2)\left(\frac{1}{4} + k_2^2\right)\left(2p|k_2\, L-1\right) rR_{21}\,(r)\ . \qquad \text{(A3)}$$

$$\left[\frac{d^2}{dr^2} + k_2^2 - \frac{(L+1)(L+2)}{r^2} + \frac{2}{r}\right] u\left(k_2\, L+1,\ r\right)$$

$$= -2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1\,(1s\,2p,\ r)\, u\left(k_1\, L,\ r\right) - 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1\,(2s\,2p,\ r)\, u\left(k_2\, L,\ r\right)$$

$$- \frac{6}{5}\frac{\sqrt{L(L+1)}}{2L+1}\, y_2\,\left(2p\,2p,\ r\right) u\left(k_2\, L-1,\ r\right)$$

$$+ 2\left[y_0\,(2p\,2p,\ r) + \frac{(L+2)\, y_2\,(2p\,2p,\ r)}{5(2L+1)}\right] u\left(k_2\, L+1,\ r\right)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{10}\,(r)\, y_{L+1}\left(2p\, k_1\, L,\ r\right)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{20}\,(r)\, y_{L+1}\left(2p\, k_2\, L,\ r\right)$$

$$- \frac{6\beta\sqrt{L(L+1)}}{(2L+1)^2}\, rR_{21}\,(r)\, y_L\left(2p\, k_2\, L-1,\ r\right)$$

$$+ \frac{6\beta}{2L+3}\, rR_{21}\,(r)\left[\frac{y_L\left(2p\, k_2\, L+1,\ r\right)}{(2L+1)^2} + \frac{(L+2)\, y_{L+2}\left(2p\, k_2\, L+1,\ r\right)}{(2L+5)}\right]$$

$$- \beta\delta(L,\ 0)\left(\frac{1}{4} + k_2^2\right)\left(2p|k_2\, L+1\right) rR_{21}\,(r)\ . \tag{A4}$$

Appendix B

Elements of the Potential Matrix

Elements of D_{ij}

$$D_{11} = -\left(1+\frac{1}{r}\right)e^{-2r}, \quad D_{22} = -\left(\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{8}\right)e^{-r},$$

$$D_{33} = -\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{24}\right]e^{-r} + \frac{6(L-1)}{2L+1}\left[\frac{1}{r^3} - \left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right],$$

$$D_{44} = -\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{24}\right]e^{-r} + \frac{6(L+2)}{2L+1}\left[\frac{1}{r^3} - \left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right],$$

$$D_{12} = D_{21} = \frac{2\sqrt{2}}{9}\left(r+\frac{2}{3}\right)e^{-3/2\,r},$$

$$D_{13} = D_{31} = \frac{128\sqrt{2}}{243} \times \left(\frac{L}{2L+1}\right)^{1/2}\left[\frac{1}{r^2} - \left(\frac{1}{r^2}+\frac{3}{2r}+\frac{9}{8}+\frac{27r}{64}\right)e^{-3r/2}\right],$$

$$D_{14} = D_{41} = -\frac{128\sqrt{2}}{243}\left(\frac{L+1}{2L+1}\right)^{1/2}\left[\frac{1}{r^2} - \left(\frac{1}{r^2}+\frac{3}{2r}+\frac{9}{8}+\frac{27r}{64}\right)e^{-3r/2}\right],$$

$$D_{23} = D_{32} = -3\left(\frac{L}{2L+1}\right)^{1/2}\left[\frac{1}{r^2} - \left(\frac{1}{r^2}+\frac{1}{r}+\frac{1}{2}+\frac{r}{6}+\frac{r^2}{24}\right)e^{-r}\right],$$

$$D_{24} = D_{42} = 3\left(\frac{L+1}{2L+1}\right)^{1/2}\left[\frac{1}{r^2} - \left(\frac{1}{r^2}+\frac{1}{r}+\frac{1}{2}+\frac{r}{6}+\frac{r^2}{24}\right)e^{-r}\right],$$

$$D_{34} = D_{43} = -18\left[\frac{L(L+1)}{(2L+1)^2}\right]^{1/2}\left[\frac{1}{r^3} - \left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right].$$

Elements of F_{ij}

$$F_{11} = \frac{\beta}{2L+1}\left[\frac{R_{10}}{r^L}\int_0^r R_{10}\, r'^{L+1}\, dr' - R_{10}\, r^{L+1}\int_0^r \frac{R_{10}}{r'^L}\, dr'\right],$$

$$F_{22} = \frac{\beta}{2L+1}\left[\frac{R_{20}}{r^L}\int_0^r R_{20}\, r'^{L+1}\, dr' - R_{20}\, r^{L+1}\int_0^r \frac{R_{20}}{r'^L}\, dr'\right],$$

$$F_{33} = \frac{3\beta}{2L-1}\left[\frac{1}{(2L+1)^2}\left(\frac{R_{21}}{r^L}\int_0^r R_{21}\, r'^{L+1}\, dr' - R_{21}\, r^{L+1}\int_0^r \frac{R_{21}}{r'^L}\, dr'\right)\right.$$

$$\left. + \frac{L-1}{2L-3}\left(\frac{R_{21}}{r^{L-2}}\int_0^r R_{21}\, r'^{L-1}\, dr' - R_{21}\, r^{L-1}\int_0^r \frac{R_{21}}{r'^{L-2}}\, dr'\right)\right],$$

$$F_{44} = \frac{3\beta}{2L+3}\left[\frac{1}{(2L+1)^2}\left(\frac{R_{21}}{r^L}\int_0^r R_{21}\, r'^{L+1}\, dr' - R_{21}\, r^{L+1}\int_0^r \frac{R_{21}}{r'^L}\, dr'\right)\right.$$

$$\left. + \frac{L+2}{2L+5}\left(\frac{R_{21}}{r^{L+2}}\int_0^r R_{21}\, r'^{L+3}\, dr' - R_{21}\, r^{L+3}\int_0^r \frac{R_{21}}{r'^{L+2}}\, dr'\right)\right],$$

$$F_{12} = \frac{\beta}{2L+1}\left[\frac{R_{20}}{r^L}\int_0^r R_{10}\, r'^{L+1}\, dr' - R_{20}\, r^{L+1}\int_0^r \frac{R_{10}}{r'^L}\, dr'\right],$$

$$F_{21} = F_{12}\left[R_{10} \rightleftarrows R_{20}\right],$$

$$F_{13} = \sqrt{3}\beta\left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L-1}}\int_0^r R_{10}\, r'^L\, dr - R_{21}\, r^L\int_0^r \frac{R_{10}}{r'^{L-1}}\, dr'\right],$$

$$F_{31} = F_{13}\left[R_{10} \rightleftarrows R_{21}\right],$$

$$F_{14} = -\sqrt{3}\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L+1}}\int_0^r R_{10}\, r'^{L+2}\, dr' - R_{21}\, r^{L+2}\int_0^r \frac{R_{10}}{r'^{L+1}}\, dr'\right],$$

$$F_{41} = F_{14}\left[R_{10} \rightleftarrows R_{21}\right],$$

$$F_{23} = \sqrt{3}\beta\left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L-1}}\int_0^r R_{20}\, r'^L\, dr' - R_{21}\, r^L\int_0^r \frac{R_{20}}{r'^{L-1}}\, dr'\right],$$

$$F_{32} = F_{23}\left[R_{20} \rightleftarrows R_{21}\right],$$

$$F_{24} = -\sqrt{3}\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L+1}}\int_0^r R_{20}\, r'^{L+2}\, dr' - R_{21}\, r^{L+2}\int_0^r \frac{R_{20}}{r'^{L+1}}\, dr'\right],$$

$$F_{42} = F_{24}\left[R_{20} \rightleftarrows R_{21}\right] ,$$

$$F_{34} = -3\beta\left[\frac{L(L+1)}{(2L+1)^4}\right]^{1/2} \times \left[\frac{R_{21}}{r^L}\int_0^r R_{21}\, r'^{L+1}\, dr' - R_{21}\, r^{L+1}\int_0^r \frac{R_{21}}{r'^L}\, dr'\right] ,$$

$$F_{34} = F_{43} .$$

Elements of g_{ij} and h_{ij}

$$g_{11} = \frac{\beta R_{10}\, r^{L+1}}{2L+1} , \quad h_{11} = R_{10}\left[\frac{1}{r^L} - \frac{1+k_1^2}{2}\,\delta(L,\,0)\, r\right] ,$$

$$g_{22} = \frac{\beta R_{20}\, r^{L+1}}{2L+1} , \quad h_{22} = R_{20}\left[\frac{1}{r^L} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,\,0)\, r\right] ,$$

$$g_{33}^1 = \frac{3\beta R_{21}\, r^{L+1}}{(2L-1)(2L+1)^2} , \quad h_{33}^1 = \frac{R_{21}}{r^L} ,$$

$$g_{33}^2 = \frac{3\beta(L-1)\, R_{21}\, r^{L-1}}{(2L-1)(2L-3)} , \quad h_{33}^2 = R_{21}\left[\frac{1}{r^{L-2}} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,\,2)\, r\right] ,$$

$$g_{44}^1 = \frac{3\beta R_{21}\, r^{L+1}}{(2L+3)(2L+1)^2} , \quad h_{44}^1 = R_{21}\left[\frac{1}{r^L} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,\,0)\, r\right] ,$$

$$g_{44}^2 = \frac{3\beta(L+2)\, R_{21}\, r^{L+3}}{(2L+3)(2L+5)} , \quad h_{44}^2 = \frac{R_{21}}{r^{L+2}} ,$$

$$g_{12} = \frac{\beta}{2L+1}\, R_{20}\, r^{L+1} , \quad h_{12} = R_{10}\left[\frac{1}{r^L} - \frac{1+k_2^2}{2}\,\delta(L,\,0)\, r\right] ,$$

$$g_{21} = g_{12}\left[R_{20} \longrightarrow R_{10}\right] , \quad h_{21} = h_{12}\left[R_{10} \longrightarrow R_{20}\right] ,$$

$$g_{13} = \sqrt{3}\beta\left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} R_{21}\, r^L , \quad h_{13} = R_{10}\left[\frac{1}{r^{L-1}} - \frac{1+k_2^2}{2}\,\delta(L,\,1)\, r\right] ,$$

$$g_{31} = g_{13}\left[R_{21} \longrightarrow R_{10}\right] , \quad h_{31} = h_{13}\left[R_{10} \longrightarrow R_{21}\right] ,$$

$$g_{14} = -\sqrt{3}\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} R_{21}\, r^{L+2} , \quad h_{14} = \frac{R_{10}}{r^{L+1}} ,$$

$$g_{41} = g_{14}\left[R_{21} \longrightarrow R_{10}\right] , \quad h_{41} = h_{14}\left[R_{10} \longrightarrow R_{21}\right] ,$$

$$g_{23} = \sqrt{3}\beta \left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} R_{21}\, r^L , \quad h_{23} = R_{20}\left[\frac{1}{r^{L-1}} - \frac{\frac{1}{4} + k_2^2}{2}\, \delta(L, 1)\, r\right] ,$$

$$g_{32} = g_{23}\left[R_{21} \longrightarrow R_{20}\right] , \quad h_{32} = h_{23}\left[R_{20} \longrightarrow R_{21}\right] ,$$

$$g_{24} = -\sqrt{3}\beta \left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} R_{21}\, r^{L+2} , \quad h_{24} = \frac{R_{20}}{r^{L+1}} ,$$

$$g_{42} = g_{24}\left[R_{21} \longrightarrow R_{20}\right] , \quad h_{42} = h_{24}\left[R_{20} \longrightarrow R_{21}\right] ,$$

$$g_{34} = -3\beta \left[\frac{L(L+1)}{(2L+1)^4}\right]^{1/2} R_{21}\, r^{L+1} , \quad h_{34} = \frac{R_{21}}{r^L} ,$$

$$g_{43} = g_{34} .$$

In the F_{ij} matrix the interchange of the functions R_{10}, R_{20}, and R_{21} accompanies the interchange of their arguments too.

Appendix C

Removal of the Singularity in the Determinant of the Coefficients of the Linear Transformation for L = 0, 1

Case I: L = 0

By using the definition of D_{ij} and F_{ij} and Equations 63 in the text, the following relation can be derived from Equation 59 (text):

$$\int_0^\infty \left[rR_{20}\left(\frac{d^2}{dr^2} + k_1^2\right) v_1 - \beta\, rR_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_2 \right] dr = -\frac{2}{\sqrt{3}}\left[a_{13}\, B_{24} - \beta\, a_{23}\, B_{14}\right] , \tag{C1}$$

where the superscript μ is suppressed when there is only one value for μ, and

$$a_{13} = \int_0^\infty R_{10}\, R_{21}\, r^3\, dr = \left[2^{15} \times 3^{-9}\right]^{1/2} ,$$

$$a_{23} = \int_0^\infty R_{20}\, R_{21}\, r^3\, dr = -\,3\sqrt{3} .$$

Integrating the left-hand side of Equation C1 by parts, and making use of Equations 11 and 63 (text), we obtain

$$\int_0^\infty \left[rR_{20}\left(\frac{d^2}{dr^2} + k_1^2\right) v_1 - \beta\, rR_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_2 \right] dr = -\,2\left[B_{21} - \beta B_{12}\right] . \tag{C2}$$

We conclude that

$$B_{21} - \beta B_{12} = \frac{1}{\sqrt{3}}\left[a_{13} B_{24} - \beta\, a_{23} B_{14}\right] . \tag{C3}$$

Equation C3 connects the right-hand sides of the four equations of Equation 62 specified by $ij = 21,\ 12,\ 24,\ 14$. A similar relation should hold among the left-hand sides of these equations. This in fact is the case and, by making use of the first of Equations 63, it can be shown directly that equations similar to Equation C3 hold among the elements of each column $kl\nu$ of the left-hand side of Equation 62 specified by $ij = 21,\ 12,\ 24,\ 14$. We conclude that one equation of Equation 62 is linearly dependent on others and the determinant of Equation 62 is singular.

Case II: L = 1

Similar to the previous case, the following relation can be derived from Equation 59 in the text:

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2} + k_1^2 - \frac{2}{r^2}\right) v_1 - \beta\, rR_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3 \right] dr$$

$$= -\frac{2}{3}\left[\beta a_{13} B_{11} + \beta a_{23} B_{12} - a_{13} B_{33}^1 + \sqrt{2}\left(a_{13} B_{34} - \frac{3}{5}\beta a_{33} B_{14}\right)\right] , \tag{C4}$$

where

$$a_{33} = \int_0^\infty R_{21}^2\, r^4\, dr = 30 .$$

Integrating the left-hand side of Equation C4 by parts, and making use of Equations 11 and 63, we obtain

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2} + k_1^2 - \frac{2}{r^2}\right) v_1 - \beta\, rR_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3 \right] dr = -2\left[B_{31} - \beta B_{13}\right] . \tag{C5}$$

Combining Equations C4 and C5, we get

$$B_{31} - \beta B_{13} = \frac{1}{3}\left[\beta a_{13} B_{11} + \beta a_{23} B_{12} - a_{13} B_{33}^1 + \sqrt{2}\left(a_{13} B_{34} - \frac{3}{5}\beta a_{33} B_{14}\right)\right] . \tag{C6}$$

Finally, Equation 59 (text) gives the following relation:

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2} + k_2^2 - \frac{2}{r^2}\right) v_2 - \beta\, rR_{20}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3 \right] dr$$

$$= -\frac{2}{3}\left[\beta a_{23} B_{22} + \beta a_{13} B_{21} - a_{23} B_{33}^1 + \sqrt{2}\left(a_{23} B_{34} - \frac{3}{5}\beta a_{33} B_{24}\right)\right] . \tag{C7}$$

Integration by parts of the left-hand side gives, as before,

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2} + k_2^2 - \frac{2}{r^2}\right) v_2 - \beta\, rR_{20}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3 \right] dr = -2\left[B_{32} - \beta B_{23}\right] , \tag{C8}$$

whereupon we get

$$B_{32} - \beta B_{23} = \frac{1}{3}\left[\beta a_{23} B_{22} + \beta a_{13} B_{21} - a_{23} B_{33}^{1} + \sqrt{2}\left(a_{23} B_{34} - \frac{3}{5}\beta a_{33} B_{24}\right)\right] . \tag{C9}$$

Similar to the case $L = 0$, Equations C6 and C9 indicate that two equations of Equation 62 are linearly dependent on others and the determinant of Equation 62 is singular.

To remove the singularity in the $L = 0$ case, one of the C_{kl}^{ν} is chosen to be arbitrary; and a degenerate equation is removed from Equation 62 (text). Similarly, in the $L = 1$ case two of the C_{kl}^{ν} are chosen arbitrary; and two degenerate equations are removed from Equation 62.

Appendix D

Elements of the Matrix of the Sum of the Asymptotic Coulomb and Centrifugal Potentials

$$U_{11} = L(L+1)\,r^{-2}, \qquad U_{22} = L(L+1)\,r^{-2},$$

$$U_{33} = (L-1)\,Lr^{-2} + 12(L-1)\,(2L+1)^{-1}\,r^{-3}, \qquad U_{44} = (L+1)\,(L+2)\,r^{-2} + 12(L+2)\,(2L+1)^{-1}\,r^{-3},$$

$$U_{12} = U_{21} = 0, \quad U_{13} = U_{31} = \left[\frac{256\sqrt{2}}{243}\right]\left[\frac{L}{(2L+1)}\right]^{1/2} r^{-2},$$

$$U_{14} = U_{41} = -\left[\frac{256\sqrt{2}}{243}\right]\left[\frac{(L+1)}{(2L+1)}\right]^{1/2} r^{-2}, \qquad U_{23} = U_{32} = -6\left[\frac{L}{(2L+1)}\right]^{1/2} r^{-2},$$

$$U_{24} = U_{42} = 6\left[\frac{(L+1)}{(2L+1)}\right]^{1/2} r^{-2}, \qquad U_{34} = U_{43} = -36\left[L(L+1)\right]^{1/2}(2L+1)^{-1}\,r^{-3}.$$

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